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TECHNICAL ABSTRACTS

COFIRING BIOMASS IN COAL BOILERS: PILOT AND UTILITY SCALE EXPERIENCES

L.L. Baxter, M. Rumminger and T. Lind, Sandia National Laboratories, Livermore, CA 94550 e-mail: baxter@sandia.gov, D. Tillman, Foster Wheeler Development Corporation, and E. Hughes, Electric Power Research Institute (to be Presented at the *1st World Conference and Technology Exhibition*, Held in Seville, Spain, June 1999).

Experiences and guidelines for cofiring biomass with coal in pulverized coal boilers are reviewed for a range of fuels and under a variety of conditions. Issues of ash deposition, corrosion, pollutant formation, char burnout, boiler efficiency and fuel preparation are reviewed. Pilot-scale investigations covering a wide range of cofiring fractions, fuels and conditions are shown to be similar to available utility-scale data. The data suggest that ash deposits from many wood residues will be manageable, at times even more manageable than for pure coal combustion. However, ash deposits from agricultural residues and energy crops range from similar to those from coal to far less manageable than those from coal. Corrosion rates from fuel chlorine are shown to be somewhat abated by the reactions between (mainly coal-derived) sulfur and (mainly biomass-derived) chlorides. Proper choices of coal and biomass allow corrosion to be managed. Sulfur dioxide emissions are shown to be almost universally decreased by cofiring while NO_x emissions are generally decreased when cofiring low-nitrogen fuels (wood residues). Particles less than about 3 mm are shown to completely burn within the residence time in the boiler while larger or high-moisture fuels are increasingly difficult to burn. Boiler efficiency (on a higher-heating-value-basis) decreases slightly with most biomass fuels due to a combination of fuel moisture and increased parasitic losses such as ID fan and fuel preparation loads. Fuel preparation is shown to be a major issue in successful implementation of cofiring systems, with preparation criteria including top particle size of ¼ inch, maximum moisture content of about 50%, and feeding systems ranging from joint injection to dedicated feed lines. Dedicated feed lines are generally required for cofiring percentages above 5-10% (by mass) for both pulverizer pluggage and fuel handling issues. Capital costs of installing cofiring systems ranges from $50 to $250 per kW of biomass capacity. Operating and fuel costs are highly variable. In general, cofiring biomass with coal is seen as the most cost effective and lowest risk way to increase renewable energy as a fraction of total power production.

ENGINEERING MODELS OF BIOMASS COMBUSTION PROCESSES
L.L. Baxter, Sandia National Laboratories, Livermore, CA 94550, e-mail: baxter@sandia.gov, A. Robinson, Carnegie Mellon University, and S. Buckley, University of Maryland (to be Presented at the *1st World Conference and Technology Exhibition*, Held in Seville, Spain, June 1999).

Experimental data and theoretical analyses are presented that outline essential features of biomass combustion, including heating and drying, devolatilization, and char oxidation. Relatively advanced model approaches for describing the mass loss history of biomass particles are compared with data collected from several highly instrumented furnaces. Models account for particle size and density, shape, internal temperature gradients, and composition. Data are collected using a combination of *in situ* and *ex situ* diagnostics. Individual particle size, shape, and temperature are monitored as a function of time during combustion in environments typical of industrial furnaces. Particle mass loss and composition are monitored for collections of particles as a function of residence time and gas conditions (composition and temperature). These data are analyzed using robust engineering models of kinetics, heat transfer, and mass transfer. Drying and devolatilization are found to primarily heat-transfer controlled whereas oxidation is found to be primarily mass-transfer controlled for most biomass of practical concern.

DETAILED COMBUSTION MODELING AS AN AID TO PROPELLANT FORMULATION: TWO NEW STRATEGIES
M.S. Miller and W.R. Anderson, Weapons and Materials Research Directorate, Army Research Laboratory, Aberdeen Proving Ground, MD 21005 (Army Research Laboratory, Final Report ARL-TR-2167, 41 pp., March 2000).

There has been considerable progress recently in the development and use of elementary chemical-reaction mechanisms to describe the gas-phase energy release of energetic materials. Such advances present an opportunity to examine the extent to which these models might be used to provide guidance to the propellant formulator. In this report, we develop two methodologies that may prove helpful to the development of propellant formulations with tailored combustion characteristics. First, the dependence of the burning rate on the path of condensed-phase decomposition was computed for nitroglycerine (NG) combustion. It was found that some sets of decomposition products lead to nearly an order of magnitude higher burning rate than is observed experimentally. This indicates that efforts to influence the path of decomposition might be a novel and powerful approach to tailoring burning rate. Second, a methodology for calculating the effectiveness of different chemical additives on the burning rate was developed and demonstrated for several chemical additives added to NG. Burning rates were calculated for the additives H_2, CH_2O, and NH_3 and flame-structure calculations made for HNCO as an additive. NH_3 accelerates the burning rate of NG, and HNCO is expected to retard it; both reduce the dark-zone length and thus may reduce ignition delays in guns.

VARIATION OF EQUIVALENCE RATIO AND ELEMENT RATIOS IN LOW PRESSURE PREMIXED FLAMES OF ALIPHATIC FUELS
C.J. Pope and J.A. Miller, Sandia National Laboratories, Livermore, CA 94550 (Presented at the *Western States Section Meeting of the Combustion Institute*, Held in Golden CO, March 2000).

In previously published work it was found that the element ratios (such as C/O, H/O, H/C) and the equivalence ratio all varied in the flame zone of a low pressure premixed fuel-rich benzene/oxygen/argon laminar flat flame. These variations were seen from analyses of both the data and detailed kinetic modeling. In the present work, seven additional flames were analyzed in the same manner, including five flames with a single hydrocarbon fuel (methane, acetylene, ethylene, allene and propene) and two flames with a mixture of fuels (acetylene/allene, hydrogen/allene). All the flames had argon as the diluent, with pressures between 20 and 37.5 torr, equivalence ratios between 1.6 and 2.5, cold gas velocities between 42 and 126 cm/s.

All of these flames showed variations in the element ratios and equivalence ratios. Furthermore, these variations changed in a consistent pattern with respect to the molecular weight of the fuel. In the flame zone, the percent change in the H/O, C/O and equivalence ratios increased with increasing molecular weight of the fuel, except for the hydrogen/allene flame in which the C/O ratio first increases, then decreases in the flame zone. Also, unlike all the other hydrocarbon flames, the C/O ratio decreases below its inlet value for the methane flame. The H/O and equivalence ratios decrease below their inlet values for the hydrogen/allene flame. These results are explained in terms of differential diffusion effects between the products and the reactants, which increase as the fuel becomes increasingly heavier than the major carbon- and hydrogen-containing products.

A FLAME EMBEDDING MODEL FOR TURBULENT COMBUSTION SIMULATION

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Combustion in a turbulent flow may take the form of a thin, continuous flame surface convolved by vortical structures. The flame embedding approach for this regime of turbulent combustion seeks to decouple the flame surface from non-reacting portions of the flow, providing for more computationally efficient simulation. An accurate subgrid model for the combustion zone - for the dynamic effect of strain on the burning of the flame surface - is thus an essential component of the flame and embedding approach. This paper presents an unsteady one-dimensional strained flame model incorporating detailed chemical kinetics and transport. A novel numerical formulation, based on a globalized inexact Newton method and a preconditioned Krylov subspace linear solver, ensure efficient and robust convergence despite the stiffness of detailed chemistry. The model is validated via comparison with a well-benchmarked steady-state strained flame code, then studied in the context of flame embedding: A two-dimensional direct numerical simulation of a premixed flame interacting with a vortex pair is presented, and the one-dimensional model is used to characterize the burning of the flame surface under the same imposed strain conditions. This example leads to a redefinition of the appropriate strain to be used with the subgrid model, particularly as the flame thickness approaches the length scale of vortical structures in the flow. The discussion thus points to an extension of the applicability of the model beyond the traditional flamelet regime.

STABILITY OF QUASI-STEADY DEFLAGRATIONS IN CONFINED POROUS ENERGETIC MATERIALS

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Previous analyses have shown that unconfined deflagrations propagating through both porous and nonporous energetic materials can exhibit a thermal/diffusive instability that corresponds to the onset of various oscillatory modes of combustion. For porous materials, two-phase-flow effects, associated with the motion of the gas products relative to the condensed material, play a significant role that can shift stability boundaries with respect to those associated with the nonporous problem. In the present work, additional significant effects are shown to be associated with confinement, which produces an overpressure in the burned-gas region that leads to reversal of the gas flow and hence partial permeation of the hot gases into the unburned porous material. This results in a superadiabatic effect that increases the combustion temperature and, consequently, the burning rate. Under the assumption of gas-phase quasi-steadiness, an asymptotic model is presented that facilitates a perturbation analysis of both the basic solution, corresponding to a steadily propagating planar combustion wave, and its stability. The neutral stability boundaries collapse to the previous results in the absence of confinement, but different trends arising from the presence of the gas-permeation layer are predicted for the confined problem. Whereas two-phase-flow effects are generally destabilizing in the unconfined geometry, the effects of increasing overpressure and hence combustion temperature associated with confinement are shown to be generally stabilizing with respect to thermal/diffusive instability, analogous to the effects of decreasing heat losses on combustion temperature and stability in single-phase deflagrations.

MODELING PHOTOCHEMICAL ISOTOPE FRACTIONATION OF STRATOSPHERIC TRACE GASES

M.C. McCarthy and K.A. Boering, College of Chemistry, University of California, Berkeley, CA 94720, and P.S. Connell and D.A. Rotman, Atmospheric Sciences Division, Lawrence Livermore National Laboratory, Livermore, CA 94550 (Presented at the *219th National Meeting of the American Chemical Society*, Held in San Francisco CA, March 2000).

Observations, laboratory experiments, and theoretical work have demonstrated the significant photochemical isotope fractionation that occurs in the stratosphere for a number of chemically and radiatively important trace species, including O_3, CO_2, CH_4, and N_2O, yet global-scale isotope variations remain largely unexplored and unquantified. The nature of the photochemical isotope fractionation ranges from simple (for example, faster rates of photolytic destruction for the light isotopomers of N_2O and CH_4) to complex (for example, mass-independent fractionation of oxygen isotopes in O_3 and CO_2, the chemical physics of which is still under debate). Current experimental and theoretical isotope-specific reaction and photolysis rates are being incorporated into the Livermore 2-D model in order to test understanding of the underlying fractionation mechanisms. These calculations will help to determine the potential for variations in isotope compositions to be used in quantifying stratospheric chemistry and mass transport processes and the degree to which the large fractionations in the stratosphere may affect free tropospheric isotopic compositions. Model results for CH_4 and other species will be presented and compared with observations, and their application to stratospheric chemistry and the sources and sinks of greenhouse gases will be discussed.

OXYGEN ISOTOPE EFFECTS IN THE PRODUCTION AND REMOVAL OF ATMOSPHERIC CARBON MONOXIDE

R.E. Weston, Chemistry Department, Brookhaven National Laboratory, P.O. Box 5000, Upton, NY 11973 (Presented at the *219th National Meeting of the American Chemical Society*, Held in San Francisco CA, March 2000).

A substantial fraction of atmospheric carbon monoxide results from the oxidation of methane and other natural hydrocarbons. Based on the overall ^{18}O abundance and the budget of atmospheric CO, various authors have proposed that carbon monoxide produced from methane oxidation has an ^{18}O abundance of $\delta^{18}O$ ranging from 15% (Stevens and Wagner, 1989) to -20% (Brenninkmeijer and Roeckmann, 1997). The mechanism of methane oxidation is examined, using recommended values of rate constants, and it is shown that the rate-determining step is the reaction CH_4+OH(or Cl)$\rightarrow CH_3+H_2O$ (or HCl). Based on this mechanism, the only step that can produce isotopic fractionation in the CO product is the reaction $CH_3+O_2\rightarrow CH_3OO$. Since atmospheric oxygen has a $\delta^{18}O$ value of 23.5, a very large kinetic isotope effect would be required to produce CO with the proposed isotopic composition. The implications of the reported anomalous kinetic isotope effect in the CO+OH reaction will also be discussed.

ANOMALOUS FRACTIONATION OF OXYGEN ISOTOPES IN STRATOSPHERIC CARBON DIOXIDE: FROM OZONE PRODUCTION AND TRANSPORT TO GLOBAL BIOSPHERIC PRODUCTIVITY

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Measurements of the oxygen isotopic composition of stratospheric carbon dioxide from whole air samples taken by the NASA ER-2 aircraft during the breakup of the 1996-97 Arctic vortex show anomalous enrichment in ^{17}O and ^{18}O (for which $d^{17}O$ $^{1}0.5*$ $d^{18}O$), as have previous measurements from several balloon and rocket flights. These results, and their correlation with simultaneous, in situ measurements of the concentrations of N_2O, O_3, and CO_2, provide new observation-based constraints on the source of the fractionation that leads to the enrichment, on the distribution of this anomalous fractionation in the stratosphere, on its use as a tracer of stratospheric chemistry and transport, and on the magnitude of the flux of the anomalous signature in CO_2 into the troposphere. Quantifying the anomalous isotopic flux to the troposphere is a prerequisite for using the isotopic composition of O_2 as an index of modern primary productivity on Earth and, through ice core studies, changes in biological productivity on glacial-interglacial time scales since the anomalous enrichment in stratospheric CO_2 results in a small anomalous depletion in O_2, which can build up over the lifetime of O_2 with respect to turnover by the biosphere.

ATMOS VERSION-3 WATER VAPOR MEASUREMENTS: COMPARISONS WITH ATMOS VERSION 2 RETRIEVALS AND OBSERVATIONS FROM TWO ER-2 LYMAN-α HYGROMETERS, MkIV, MAS, HALOE AND MLS

H.A. Michelsen, G.L. Manney, F.W. Irion, G.C. Toon, M.R. Gunson, C.P. Rinsland, R. Zander, E. Mahieu, M.J. Newchurch, P.N. Purcell, E.E. Remsberg, J.M. Russell III, H.C. Pumphrey, J.W. Waters, R.M. Bevilacqua, K.K. Kelly, and C.R. Webster (to Appear in the *Journal of Geophysical Research*).

We have compared a new version of ATMOS retrievals (Version 3) of stratospheric and mesospheric water vapor with observations from satellite-, balloon-, and aircraft-borne instruments. ATMOS Version 3 water vapor measurements demonstrate agreement to within 5% with observations from the MkIV balloon-borne instrument in the middle and lower stratosphere. In the middle and upper stratosphere, agreement is within 5% with the MAS shuttle-borne instrument and within 10% with the HALOE (Version 19) satellite instrument. Agreement with both MAS and HALOE is within 30% in the lower stratosphere and mesosphere. ATMOS agrees with the NOAA Lyman-α hygrometer to within 5%, except when features with spatial scales less than the vertical resolution of ATMOS (such as the lower stratospheric seasonal cycle) are prevalent. ATMOS observations are 11-16% dryer than measurements from the Harvard Lyman-α hygrometer and 10-15% wetter than those from the MLS (prototype Version 0104) satellite instrument. Version 3 water vapor retrievals produce mixing ratios of H_2O in the upper stratosphere and lower mesosphere that are typically 5-10% lower than values produced by Version 2 retrievals between 1 and 0.05 mbar and are thus in better agreement with HALOE observations.

FEATURES AND TRENDS IN ATMOS VERSION 3 WATER VAPOR AND METHANE MEASUREMENTS

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Mixing ratios of water vapor entering the stratosphere are inferred from the ATMOS measurements to be 3.25(±0.42) ppm in 1985, 3.53(±0.45) ppm in 1992, and 3.67(±0.46) ppm in 1993 and 1994, yielding an average increase of 0.047(±0.007) ppm/yr or 1.4%/yr between 1985 and 1994 (1σerror). Strong evidence for a seasonal cycle in water vapor is apparent below 45 km in the tropics, and vertical ascent rates inferred from these tropical profiles are consistent with previous estimates. An enhancement in the sum $[H_2O]+2[CH_4]$ apparent between 45 and 60 km in the tropics appears to be consistent with remnants of a seasonal cycle in $[H_2O]$.

PHOTOINDUCED ISOTOPIC FRACTIONATION OF STRATOSPHERIC NITROUS OXIDE

C.E. Miller, Department of Chemistry, Haverford College, 370 Lancaster Avenue, Haverford, PA 19041 (Presented at the *219th National Meeting of the American Chemical Society*, Held in San Francisco CA, March 2000).

Selwyn and Johnston [*J. Chem. Phys.* 74, 3791 (1981)] measured the temperature and isotopomer dependent ultraviolet absorption cross sections of N_2O for use in modeling stratospheric photochemistry. This poster demonstrates how isotopomer dependent photodissociation rates account for the isotopic fractionation observed in stratospheric N_2O and a rapidly growing number of laboratory experiments. Photoinduced Isotopic Fractionation Effects, or PHIFE, explain the distinct fractionation signatures found for $^{15}N/^{14}N$, $^{18}O/^{16}O$, $^{17}O/^{18}O$ and $^{15}N/^{18}O$ ratios in both laboratory and remote sensing measurements. Furthermore, PHIFE predicts substantially different isotopic fractionations in the stratosphere for the isotopomers $^{15}N^{14}N^{16}O$ and $^{14}N^{15}N^{16}O$ which have identical molecular weights but different isotopic substitution sites. Modeling results based on this theory suggest that there is no demonstrable reason to invoke a significant chemical source of N_2O in the middle atmosphere and that N_2O multi-isotope correlations should prove a useful measure of stratospheric air parcel history.

VAPORIZATION, TRANSPORT, AND DEPOSITION OF SODIUM VAPOR SPECIES IN OXYGEN-NATURAL GAS-FIRED SODA-LIME-SILICA GLASS MELTING FURNACES

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Measurements and calculations were performed to better understand the processes by which sodium species vaporized from the surface of molten soda-lime-silica glass contribute to corrosion of silica refractory in melting furnaces and why higher corrosion rates are sometimes observed when oxygen is used instead of air for combustion of natural gas. Line-of-sight measurements of gas temperature and sodium atom concentration were made across the combustion space in a full scale oxygen-natural gas-fired glass furnace by emission-absorption pyrometry and spectrometry using the atomic sodium D-lines at 589 nm. Gas temperatures, except near the cooler raw material feed, were near 1700 °C. The only important sodium vapor species under the conditions investigated were sodium atoms (2.3-18 mol%) and sodium hydroxide. The total sodium, assuming chemical equilibrium, was between 95 and 136 mol ppm, nearly uniform along the length of the furnace at an average value of 120 mol ppm.
The flow of furnace gas over the glass was treated as if it were simliar to that over a flat plate, but with sufficient recirculation to appear well mixed. According to this model, the most important influences on the free stream sodium concentration are the mean glass surface temperature and surface temperature distribution. The calculated ratio of the total sodium concentration during oxygen firing to that during air firing was 3.4, in good agreement with reported observations, due to approximately equal effects of the reduced gas volume and increased water vapor content of the oxygen-natural gas combustion products. Deposition of sodium on the silica refractory of the furnace crown is expected only when the free stream sodium hydroxide concentration exceeds the equilibrium partial pressure of sodium hydroxide over the soda-silica corrosion product, at refractory temperatures approximately 200 °C below the mean temperature of the glass surface. Below this critical temperature, rates of deposition and corrosion increase with decreasing refractory temperature in the presence of a fixed distribution of glass temperatures. Maximum corrosion rates in oxygen-fired furnaces were predicted to be 1.8 times the rates in otherwise identical air-fired furnaces, due entirely to the effect of the increased water vapor content of the combustion products, and to affect a larger area of the crown. Corrosion rates are expected to decrease with increasing height of the combustion space, supporting this approach to the reduction of rates of refractory corrosion.

EXPERIMENTAL MEASUREMENTS OF THE THERMAL CONDUCTIVITY OF ASH DEPOSITS. I. MEASUREMENT TECHNIQUE

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This paper describes a technique developed to make in situ, time-resolved measurements of the effective thermal conductivity of ash deposits formed under conditions that closely replicate those found in the convective pass of a commercial boiler. Since ash deposit thermal conductivity is thought to be strongly dependent on deposit microstructure, the technique is designed to minimize the disturbance of the natural deposit microstructure. Experiments are described that demonstrate the technique, quantify experimental uncertainty, and determine the thermal conductivity of highly porous, unsintered deposits. The average measured thermal conductivity of loose, unsintered deposits is 0.14(±0.03) W/(m K), approximately midway between rational theoretical limits.

EXPERIMENTAL MEASUREMENTS OF THE THERMAL CONDUCTIVITY OF ASH DEPOSITS. II. EFFECTS OF SINTERING AND DEPOSIT MICROSTRUCTURE

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We report results from an experimental study that examines the influence of sintering and microstructure on ash deposit thermal conductivity. The initial stages of sintering and densification are accompanied by an increase in deposit thermal conductivity. Subsequent sintering continues to densify the deposit, but has little effect on deposit thermal conductivity. SEM analyses indicate that sintering creates a layered deposit structure with a relatively unsintered innermost layer. We hypothesize that this unsintered layer largely determines the overall deposit thermal conductivity. A theoretical model that treats a deposit as a two-layered material predicts the observed trends in thermal conductivity.

SPECTROSCOPY AND DYNAMICS OF THE d_2-METHOXY RADICAL, CHD_2O

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CHD_2O radicals were produced by 355 nm photolysis of CHD_2ONO seeded in argon. Supersonic jet expansion cooled the radicals rotationally and the fluorescence-excitation spectrum was probed by a frequency-doubled dye laser 2.5 cm downstream. The band origin of the spectrum was detected near 31610 cm^{-1} and many vibrational progressions were observed up to 36000 cm^{-1}. Spectra of both the $E_{3/2}$ and the higher-lying $E_{1/2}$ electronic ground states were recorded under different conditions in the jet. The C-H stretch is only weakly Franck-Condon active and hence its energy levels are difficult to access via electronic transitions. Infrared excitation detected by fluorescence depletion spectroscopy was used to populate the C-H rovibrational energy levels in the ground electronic state. Individual rovibronic fluorescence-excitation transitions of the 3^1 band were chosen for detection of ground-state depletion by an infrared laser. In this double resonance spectroscopy, first an infrared laser (Optical Parametric Oscillator (OPO) or a Raman-shifted dye laser) pulse passes through the jet and then an ultraviolet excitation laser is focused along the same path. Depletion in the fluorescence signal occurs whenever the infrared laser transfers population to an excited C-H stretching energy level. Hence, by scanning the OPO laser, an infrared absorption spectrum is obtained for the rotational state pumped by the ultraviolet laser. Many vibrational bands throughout the fundamental (2750-3000 cm^{-1}) and first overtone (5350-5500 cm^{-1}) regions of the C-H stretch have been observed using this method. Each of these bands showed different and complex rotational structures. The CHD_2O radical exhibits Jahn-Teller activity and at high energies, Coriolis resonances may also become important. This makes both vibrational and rotational assignments very difficult. Work is in progress to record the dynamically interesting second overtone region of the C-H stretch around 8000 cm^{-1} that is about 1000 cm^{-1} above the asymptotic barrier to dissociation of CHD_2O to CD_2O/CHDO and H/D.

Kinetics of Formation and Absorption Cross Section of the ClO Dimer

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The technique of Flash Photolysis with Ultraviolet Absorption Spectroscopy has been used to study the formation of Cl_2O_2 from the self-reaction of ClO radicals. Three separate monochromator/ photomultiplier tube absorption channels were used to follow the time-dependent evolution of both ClO and Cl_2O_2. ClO radicals were quantified using the differential spectroscopy technique, via simultaneous measurement of the ClO absorption at the (12,0) band peak and the adjacent valley of the (A-X) transition at approximately 275 nm. The concentration of ClO could thus be unequivocally determined in the presence of other absorbing species. The third detection channel was used to monitor the formation of Cl_2O_2 at lower wavelengths. Kinetic fitting to the ClO decay permitted comparison of the calculated yield of Cl_2O_2 with that measured using literature dimer cross sections. Experiments were performed over a range of conditions (temperature, pressure) relevant to the middle atmosphere, and the results obtained are compared with those from other recent laboratory studies.

Reaction of $O(^1D)$ with SiH_4

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In the past several decades, it has been fully demonstrated that the reaction probability depends not only on collision energies, internal excitations and impact parameters, but also on the orientation of molecules. But reactions with several product channels, the initial conditions mentioned above, will also affect the nature of reaction intermediates involved and branching ratios of various products.

In the reaction of $O(^1D)+SiH_4$, it is very interesting to find that the formation of OH is scattered forward, H_3SiO is scattered backward, and the formations of H_2SiO and SiO are forward backward symmetric. The results imply that there are three reaction intermediates involved depending on the impact parameter and the orientation of SiH_4 molecules. First two channels are direct reactions, abstraction and substitution of H atom from SiH_4. However, the formations of H_2SiO and SiO are found to go through the collision complex H_3SiOH, with subsequent elimination of one or two H_2 molecules.

Near Infrared Linestrength Measurements of Hydroperoxy Radicals

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Hydroperoxy (HO_2) radicals play crucial roles in atmospheric chemistry as a reservoir species of hydroxyl (OH) radicals. In situ, direct monitoring of HO_2 radicals under pertinent atmospheric conditions provide important clues to assessing the importance of different atmospheric reactions that take place and in testing and refining atmospheric reaction models. Concurrent laboratory measurement of HO_2 reaction rates are also important in order to build a database of reaction rates which are needed for the atmospheric reaction modeling. Spectroscopic detection of HO_2 radical in the ultraviolet is complicated by the broad, featureless absorption due to predissociation. Line strengths of HO_2 in mid-infrared vibrational bands have been characterized before, but may not be strong enough to allow ambient monitoring of HO_2. The cryogenic cooling required to operate the mid-infrared diode lasers and detectors add complexity and bulk to the in situ measurement effort as well. The low-lying electronic transition and vibrational overtone bands of HO_2 occur in the near-infrared, which offer the convenience of room temperature operated, tunable diode laser sources and photodiode detectors. We have been studying near-infrared line strengths of HO_2 radicals in the overtone band at 1.5 μm as well as transitions within low-lying electronic band near 1.42 μm. Recently, we have performed a side-by-side comparison of transitions within these two bands using DFB (Distributed Feed-Back) diode lasers that operate at room temperatures. Latest experimental results of near-infrared line strength comparisons along with a summary of previous absolute line strength measurements in the near-infrared will be reported.

Absolute CH Radical Concentrations in Rich Low-Pressure Methane/Oxygen/Argon Flames via Cavity Ringdown Spectroscopy of the $(A^2D\text{-}X^2P)$ Transition

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We measure absolute methylidyne (CH) radical concentrations in a series of rich 31.0 torr (4.13 kPa) methane/oxygen/argon flames using cavity ringdown spectroscopy. Probing via the $CH(A^2\Delta\text{-}X^2\Pi)$ transition near 430 nm gives a sensitivity of $3\text{x}10^9$ cm^{-3} for our experimental conditions, yielding a signal-to-noise ratio greater than 1000 for the strongest transitions observed. We measure profiles of CH mole fraction as a function of height above a flat-flame burner for rich flames with equivalence ratios of 1.0, 1.2, 1.4 and 1.6. These flames are modeled using the following mechanisms: 1) the GRI Mech 2.11, 2) a mechanism by Prada and Miller, 3) a modified GRI 2.11 mechanism, which employs a more realistic increased $CH+O_2$ rate coefficient, and 4) the new GRI Mech. 3.0. Generally good agreement between the models and the data is found, with the GRI 3.0 and modified 2.11 mechanism best reproducing the data. The greatest discrepancies are observed at the richest stoichiometry, where all of the models predict a wider CH profile shifted further from the burner than experimentally observed.

Laser Induced Dispersed Fluorescence Detection of Polycyclic Aromatic Compounds in Soil Extracts Separated by Capillary Electrochromatography

M.G. Garguilo, D.H. Thomas, D.S. Anex and D.J. Rakestraw, Sandia National Laboratories, Livermore, CA 94550 (to Appear in the *Journal of Chromatography A*).

Polycyclic aromatic hydrocarbons (PAHs) and nitrogen containing aromatic compounds (NCACs) are characterized in soil extracts and laboratory standards by capillary electrochromatography (CEC) with laser induced dispersed fluorescence (LIDF) detection using a liquid-nitrogen cooled charge-coupled device detector. The LIDF detection technique provides information on compound identity and, when coupled with the high resolving power of the CEC technique, proves useful in the analysis of complex mixtures. Differences in fluorescence spectra also provide a means of identifying co-eluting compounds by using deconvolution algorithms. Integration over the appropriate emission wavelength ranges for individual PAHs allows the direct comparison of detection limits obtained with LIDF detection to those obtained using laser induced fluorescence (LIF) detection by non-dispersive techniques. Detection limits range from $(0.5\text{-}96)10^{-10}$ M for selected PAHs and $(0.9\text{-}3.7)10^{-10}$ M for selected NCACs using LIDF detection. Soil extracts are also injected directly onto the CEC column to evaluate chromatographic method performance with respect to complex samples and the ability to withstand exposure to environmental samples.

DETECTION OF NITROUS ACID BY CAVITY RINGDOWN LASER ABSORPTION SPECTROSCOPY

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Cavity ringdown laser absorption spectroscopy (CRDLAS) has been utilized to detect nitrous acid (HONO) in the near ultraviolet region. A high purity HONO source (free of NO_2) has been constructed for this purpose. HONO can be detected with a low limit of 40 parts per billion at the maximum absorption wavelength and a high limit of 10 parts per million at a low absorption wavelength. A large detection dynamic range with a good linearity of absorbance vs. concentration has been demonstrated. Absorption cross sections at two wavelengths (354.3 and 352.5 nm) have been examined. Improvements of the detection sensitivity with upgraded optics and data acquisition electronics are discussed. CRDLAS provides a promising sensitive detection tool for nitrous acid in laboratory studies and real-time ambient measurements.

RELATING STATE-DEPENDENT CROSS SECTIONS TO NON-ARRHENIUS BEHAVIOR FOR THE $Cl+CH_4$ REACTION

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Thermal rate constant measurements have been used extensively to extract information about mechanisms for simple chemical reactions. In the early 1960's, Johnston and co-workers performed pioneering studies relating kinetic data with potential energy surfaces for $Cl+CH_4$ and other photochlorination reactions. In the following decades, studies of thermal rate constants for $Cl+CH_4$ have demonstrated non-Arrhenius behavior. Recent measurements of vibrational state-dependent cross sections have shown that excitation of the asymmetric stretch of CH_4 can significantly enhance the reaction rate. We have used these measurements to assess the contribution of vibrationally excited CH_4 to the non-Arrhenius behavior observed. The results of the chemical dynamics studies are consistent with the reaction rates measured between 180 and 800 K and may allow us to extrapolate the kinetics observations to experimentally difficult temperature regimes. Our conclusions have significant implications for the role of $Cl+CH_4$ in combustion and atmospheric processes.

REACTION DYNAMICS OF VIBRATIONALLY EXCITED MOLECULES: $Cl+CH_4(n_3=1)$ AND $Cl+HD(v=1)$

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We present results from our investigation of the gas phase reactions of ground state atomic chlorine with vibrationally excited methane and HD. Product differential cross sections and internal state distributions are determined. Infrared excitation and stimulated Raman pumping are used to prepare the methane and HD reagents in specific vibrational and rotational states. By controlling the polarization of the preparation lasers, the effect on reactivity of relative reagent geometry is elucidated. HCl products from $Cl+CH_4(\nu_3=1)$ show significant vibrational excitation, with the vibrationally excited products almost entirely forward scattered. These forward-scattered products are formed primarily from "T-shaped" collision trajectories, in which the chlorine abstracts a peripheral hydrogen. In contrast, the reaction with $HD(v=1)$ results in back-scattered products formed from "head-on" collision geometries. The differences in dynamics can be explained in part by the different collision energies employed. We interpret the results both in terms of simple models and by comparison to detailed theoretical calculations.

ATMOSPHERIC KINETICS OF CF_3CFHO RADICAL REACTIONS

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The CF_3CFHO radical is an intermediate in the atmospheric oxidation of CF_3CFH_2 (HFC-134a), which is a replacement for CF_2Cl_2(CFC-12) in refrigeration and air conditioning. In the atmosphere the principal paths by which CF_3CFHO is removed are by reaction with O_2,

$CF_3CFHO + O_2 = CF_3C(O)F + HO_2$,

and C-C bond scission,

$CF_3CFHO = CF_3 + HC(O)F$.

The results of an experimental investigation of the kinetics of these reactions, which was done by flash photolysis with time resolved mass spectrometry, will be presented. Ab initio molecular orbital calculations have also been done, and the results will be presented.

GAS PHASE KINETIC MEASUREMENTS OF HO_2 WITH O_3 AND NO_2 USING A TURBULENT FLOW REACTOR

S.C. Herndon, D.D. Nelson, M.S. Zahniser and C.E. Kolb, Center for Atmospheric and Environmental Chemistry, Aerodyne Research, Inc., 45 Manning Road, Billerica, MA 01821, and P.W. Villalta, Mass Spectrometry Facility, University of Minnesota Cancer Center, University of Minnesota, Box 806 Mayo, 420 Delaware Street SE, Minneapolis, MN 55455 (Presented at the *219th National Meeting of the American Chemical Society*, Held in San Francisco CA, March 2000).

The reactions of HO_2 with O_3 and NO_2 have been studied over the temperature range 200 to 300 K and pressures from 50-200 torr. Infrared absorption with a tunable diode laser is used to detect isotopically labeled $H^{18}O_2$ in order to distinguish between primary and secondary reaction pathways for the HO_2 reaction with O_3. The use of the turbulent flow technique at higher pressures minimizes surface interactions with the flow tube wall to extend the temperature range below 220 K. Results of these studies will improve our understanding of ozone chemistry in the lower stratosphere and upper troposphere.

PHOTODISSOCIATION DYNAMICS OF 2-BUTYNE AT 193 nm

J.C. Robinson, W. Sun and D.M. Neumark, Department of Chemistry/Chemical Sciences Division, University of California, Lawrence Berkeley National Laboratory, 402 Latimer Hall, Neumark Group, Berkeley, CA 94720, e-mail: jcr@radon.cchem.berkeley.edu (Presented at the *219th National Meeting of the American Chemical Society*, Held in San Francisco CA, March 2000).

The photodissociation dynamics of 2-butyne ($H_3CC{=}CCH_3$) at 193 nm have been investigated using photofragment translational spectroscopy. The studies were performed on a universal crossed molecular beams apparatus in which one beam has been replaced with the output of an excimer laser operating on the ArF transition. Two channels have been identified. The dominant channel is the H-loss channel, that is the dissociation of C_4H_6 to form $C_4H_5 + H$. Competing with this channel is the methyl-loss channel, that is the production of $C_3H_3 + CH_3$ through dissociation of C_4H_6. The data provide no evidence for a channel corresponding to the loss of molecular hydrogen. These results indicate dissociation pathways that are distinct from those for 1,3-butadiene and 1,2-butadiene, two other minima on the C_4H_6 ground state potential energy surface, which we have investigated in this laboratory using 193 nm excitation.

Photodissociation Pathways of the HNCN Radical

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The photodissociation spectroscopy and dynamics of the HNCN radical have been investigated by fast beam photofragment translational spectroscopy. Both the ($B^2A'\leftarrow X^2A''$) and ($C^2A''\leftarrow X^2A''$) electronic transitions have been observed. The ($B^2A'\leftarrow X^2A''$) band displays a prominent feature at 29013 cm^{-1}, corresponding to the origin, as well as a weaker transition located about 500 cm^{-1} to the blue. The lowest member of the ($C^2A''\leftarrow X^2A''$) band is observed at 31500 cm^{-1} and shows an extended progress of about 1000 cm^{-1} attributed to the NCN symmetric stretch. Photofragment mass distributions indicate that the ($B^2A'\leftarrow X^2A''$) transition yields photofragments $HCN+N(^4S)$ while the ($C^2A''\leftarrow X^2A''$) transition produces $N_2+CH(^2\Pi)$. The translational energy distributions reveal resolved vibrational structure of the corresponding photofragments. The $P(E_T)$ distributions provide bond dissociation energies of 2.69 ($\pm$0.03) and 2.78($\pm$0.03) eV for N_2 and $N(^4S)$ loss channels, respectively, yielding $\Delta H_{f,0\,K}=3.44(\pm 0.04)$ eV.

Femtosecond Time-Resolved Photoelectron Angular Distributions Probed During Photodissociation of NO_2

J.A. Davies, R.E. Continetti, D.W. Chandler, and C.C. Hayden, Sandia National Laboratories, Livermore, CA 94550 (to Appear in *Physical Review Letters*).

Femtosecond time-resolved photoelectron angular distributions (PADs) are measured for the first time in the molecular frame of a dissociating molecule. Various stages of the dissociation process,

$$NO_2\rightarrow NO(C^2\Pi)+O(^3P),$$

are probed using ionization of the $NO(C^2\Pi)$ fragment to $NO^+(X^1\Sigma^+)$. The PADs evolve from forward-backward asymmetric with respect to the dissociation axis at short time-delays ($\leq$500 fs) to symmetric at long time delays ($\geq$1 ps). Changes in the PADs directly reflect the time-dependence separation and reorientation of the dissociating photofragments.

Long-Range Interaction and the Alignment of $O(^1D_2)$ Fragments from the State-to-State Photodynamics of Nitrous Oxide

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The photodissociation of nitrous oxide was studied around 203-205 nm preparing the parent molecule in a single rovibrational quantum state using a hexapole state-selector. The resulting photofragments $N_2(v,J)$ and $O(^1D_2)$ were quantum-state selectively detected and their angular recoil distribution was measured using ion-imaging techniques. From analysis of the polarization sensitivity of the $O(^1D_2)$ images using two different probe schemes information on the electronic alignment of the $^1D_2$ orbital is obtained. The experimental results are compared with a theoretical analysis of the long-range quadrupole-quadrupole interaction between the N_2 and $O(^1D_2)$ fragment. Qualitative agreement is observed between this semiclassical model and the experimental results. A discussion of these results in relation to ab initio surface calculations is presented.

INTERSYSTEM CROSSING AND NONADIABATIC PRODUCT CHANNELS IN THE PHOTODISSOCIATION OF N_2O_4 NEAR 200 NM

J.A. Mueller, B.F. Parsons, M.L. Morton, S.L. Curry and L.J. Butler, Department of Chemistry and the James Franck Institute, University of Chicago, 5640 S. Ellis Ave., Chicago, IL 60637, e-mail: mueller@rainbow.uchicago.edu, and J.P.D. Abbatt, Department of Geophysical Sciences, University of Chicago (Presented at the *219th National Meeting of the American Chemical Society*, Held in San Francisco CA, March 2000).

The photodissociation of N_2O_4 excited near 200 nm provides a good example of how phenomena like intersystem crossing and the breakdown of the Born-Oppenheimer approximation can alter the dynamics and expected branching between molecular photodissociation pathways. N_2O_4 dissociates in this wavelength region to give two NO_2 molecules. The adiabatic reaction coordinate for N-N bond fission involves a change in the electronic character of the wave function from $\pi_{nb,O}\pi^*_{NO2}$ to $n\sigma^*_{N-N}$, a two-electron change analogous to that found in nitric acid and nitromethane photodissociation. The very long N-N bond in N_2O_4 allows Franck-Condon access to the region of avoided crossing. Our emission spectra of the dissociating molecules probe the early-time dynamics and the electronic character of the excited state potential energy surface in the Franck-Condon region. We make tentative assignments of the NO_2 product from photofragment time-of-flight spectra. The results suggest that a portion of the excited state wave function undergoes an efficient intersystem crossing process while the remaining portion undergoes a nonadiabatic transition. Photofragment angular distribution measurements confirm that the absorption transition dipole moment lies parallel to the N-N bond.

ACETYLENE AT THE THRESHOLD OF ISOMERIZATION

M.P. Jacobson, Physical and Theoretical Chemistry Laboratory, Oxford University, South Parks Road, Oxford, OX1 3QZ, UK, e-mail: matthew.jacobson@chem.ox.ac.uk, and R.W Field, M. Silva, and Z.R. Duan, Chemistry Department, Massachusetts Institute of Technology, 77 Massachusetts Ave., Cambridge, MA 02139 (Presented at the *219th National Meeting of the American Chemical Society*, Held in San Francisco CA, March 2000).

What are the spectroscopic signatures of the onset of isomerization? The 5 cm^{-1} resolution Dispersed Fluorescence (DF) spectrum of the (S_1-S_0) electronic transition contains patterns that are repeated in spectra originating from different S_1 vibrational levels. These patterns encode perfectly specified "bright states" fractionating into "polyads." The polyads are described by a spectroscopic effective Hamiltonian matrix model. This quantum mechanical model embodies both quantum (nodal patterns) and classical (trajectories) mechanical bifurcations, most notably the appearance of a very large amplitude and stable local bender motion along the minimum energy acetylene-vinylidene isomerization path. This explains the unexpectedly long lifetime of vinylidene-like structures observed in Coulomb Explosion Imaging experiments by Vager et al. (*Phys. Rev. Lett.* 81, 3347 (1999)). *Trans*-, *cis*- and local-bend initial plucks result in diagnostically distinct fractionation patterns in the DF spectra which sample regions above and below the normal/local bend bifurcation. Some perturbed levels in the S_1 state, which resemble a local bend pluck, permit strong sampling of the barrier region along the minimum energy isomerization path. DF data sets for $^{12}C_2H_2$, $^{13}C_2H_2$ and $^{12}C_2HD$ have been recorded and analyzed.

THEORETICAL STUDY OF HYDROGEN ABSTRACTION FROM ETHANE BY SMALL RADICALS

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Quantum chemical methods and transition state theory are used to understand experimental kinetics and obtain rate equations over an extended temperature range. The reactions: $C_2H_6+X \rightarrow C_2H_5+HX$, where X=H, O, OH, NH_2, CH_3, Cl, Br were studied. Their practical importance arises from the fact that hydrogen abstraction of saturated hydrocarbons is thought to be the rate-limiting step in many combustion and atmospheric chemical processes.

The potential energy surface was computed for each reaction employing the UHF, MP2, B3LYP and QCISD(T) methods at two different basis sets: 6-311G(d,p) and 6-311++G(3df,2p) and the G2 method as well. These open-shell systems are challenging for theoretical calculations and the energy barriers computed at different levels of theory present significant differences. Transition state structures are found to be practically linear and in some cases loosely bound adducts are formed. The effects of electron correlation, basis set size, spin contamination and zero-point energy are investigated.

The calculated geometries and frequencies were used together with canonical transition state theory to fit experimental data over a wide temperature range. Tunneling is accounted for iteratively using Eckart corrections. Activation energies obtained in this way are compared with those predicted by the computational methods and with standard 3-parameter fits. We have found special treatment of the lowest vibrational frequencies is needed in order to fit the Arrhenius curvature measured for either OH or NH_2 with ethane.

OXIDATION OF SIMPLE ALCOHOLS IN SUPERCRITICAL WATER. III. FORMATION OF INTERMEDIATES FROM ETHANOL

S.F. Rice and E. Croiset, Sandia National Laboratories, Livermore, CA 94550 (to Appear in the *Industrial and Engineering Chemistry Research*).

Raman spectroscopy is used as an in situ diagnostic to measure the oxidation of ethanol by oxygen in supercritical water. An elementary reaction mechanism based on the work of Marinov is shown to predict accurately many of the experimental observations. Experimental measurements are reported at 24.5 MPa over a temperature range of 410 to 470 °C in supercritical water with reaction times ranging from 0.5-3.0 s. Concentrations of ethanol, acetaldehyde, formaldehyde, methanol, carbon monoxide, carbon dioxide, and hydrogen peroxide are measured as a function of time and temperature. The data show that the formaldehyde is the primary stable organic intermediate. An elementary reaction mechanism, modified for supercritical water conditions and supplemented with key methylperoxyl reactions is used to interpret the observations. The experimental data are consistent with the purely radical chain oxidation process represented by this mechanism. Analysis of the mechanism identifies the primary oxidation pathway proceeding through acetaldehyde with oxidation routes involving initial abstraction of the hydroxyl hydrogen or a hydrogen atom from the secondary carbon. A pathway originating from H-abstraction from the methyl group of the ethanol molecule contributes to the overall conversion to a lesser degree.

Exploring Old and New Benzene Formation Pathways in Low Pressure Premixed Flames of Aliphatic Fuels

C.J. Pope and J.A. Miller, Sandia National Laboratories, Livermore, CA 94550 (to be Presented at the *28th International Symposium on Combustion*, to be Held in Edinburgh, Scotland, August 2000).

A modeling study of benzene and phenyl radical formation is performed for three low pressure premixed laminar flat flames having an unsaturated C_2 or C_3 hydrocarbon fuel (acetylene, ethylene and propene). Predictions using three published detailed elementary-step chemical kinetics mechanisms are tested against MBMS species profile data for all three flames. The differences between the three mechanisms predictive capabilities are explored, with an emphasis on benzene formation pathways. A new chemical kinetics mechanism is created combining features of all three published mechanisms. Included in the mechanism are several novel benzene formation reactions involving combinations of radicals such as $C_2H+C_4H_5$, $C_2H_3+C_4H_3$, and $C_5H_3+CH_3$. Reactions forming fulvene (a benzene isomer) are included, such as $C_3H_3+C_3H_5$, as well as fulvene-to-benzene reactions.
Predictions using the new mechanism show virtually all of the benzene and phenyl radical to be formed by reactions of either $C_3H_3+C_3H_3$ or $C_3H_3+C_3H_5$, with the relative importance being strongly dependent upon the fuel. $C_5H_3+CH_3$ plays a minor role in fulvene formation in the acetylene flame. The $C_2H_x+C_4H_x$ reactions do not contribute noticeably to benzene or phenyl radical formation in these flames, sometimes being a major decomposition channel for either fulvene or phenyl radical. The formation pathways differ from flame to flame, $^1CH_2+C_2H_2 \leftrightarrow C_3H_3+H$ is important for all three flames.

Time-Resolved Infrared Probing of HO_2 and OH Formation in Reactions of Alkyl Radicals with O_2

E.P. Clifford, J.D. DeSain and C.A.Taatjes, Sandia National Laboratories, Livermore, CA 94550 (to be Presented at the *16th International Symposium on Gas Kinetics*, to be Held at Cambridge UK, July 2000).

The technique of laser photolysis/cw infrared frequency modulation has been applied to reactions of various alkyl radicals with molecular oxygen. The reactions are initiated by photolytic production of Cl atoms, which produce alkyl radicals by hydrogen abstraction from stable hydrocarbon precursors. The progress of the reaction is monitored in time through cw infrared frequency-modulation spectroscopy of the HO_2 and OH products. Comparison with the $Cl_2/CH_3OH/O_2$ system provides measurements of the HO_2 yield, which allows the contributions of addition and metathesis to the total rate to be determined. Biexponential time behavior of the HO_2 production in the $C_2H_5+O_2$ and $C_3H_7+O_2$ reactions allows a separation of prompt, "direct" HO_2 formation from HO_2 produced after thermal redissociation of an initial alkylperoxy adduct. The prompt HO_2 yield exhibits a smooth increase with increasing temperature, with a small positive activation energy. The total HO_2 yield, which includes contributions from the redissociation of alkylperoxy radicals, rises sharply to 100% between 575 and 675 K. Because of the separation of timescales in the HO_2 production, this rapid rise can unambiguously be assigned to alkylperoxy dissociation. The production of OH appears to be small in both ethyl and propyl$+O_2$ reactions. The reaction of cyclopropyl radicals with O_2 shows evidence of both OH and HO_2 production, presumably in association with ring opening. The results are interpreted in the context of recent ab initio and master equation calculations.

Distributed-Feedback Dye Laser for Picosecond Ultraviolet and Visible Spectroscopy

P.P. Yaney, D.A.V. Kliner, P.E. Schrader and R.L. Farrow, Sandia National Laboratories, Livermore, CA 94550 (to Appear in the *Review of Scientific Instruments*).

We describe the design and operation of a tunable laser system for use in time-resolved spectroscopic measurements in the visible and ultraviolet spectral region. A Nd:YAG-pumped distributed-feedback dye laser (DFDL) generates pulses thate are about 100 ps in duration with a nearly transform-limited linewidth (5 GHz) at a 20 Hz repetition rate. The DFDL pulses are amplified in two bow-tie amplifiers, providing pulse energies of up to 3.0 mJ; the amplified pulses may be frequency doubled to the ultraviolet spectral region, providing up to 1.0 mJ. The DFDL wavelength is computer-stabilized to within ±0.8 pm (±0.7 GHz, two standard deviations), allowing the wavelength to be stationed on an individual atomic or molecular transition or permitting continuous spectral scans to be recorded. Application of the laser system to time-resolved measurements of OH energy transfer has been demonstrated; both laser induced fluorescence and degenerate-four-wave-mixing spectra have been recorded.

ROTATIONAL STATE-TO-STATE DIFFERENTIAL CROSS SECTIONS FOR THE HCl/Ar COLLISION SYSTEM USING VELOCITY-MAPPED ION IMAGING

K.T. Lorenz and D.W. Chandler, Sandia National Laboratories, Livermore, CA 94550, and M.S. Westley, Cornell University, Ithaca, NY 14853 (to Appear in *Physical Chemistry Chemical Physics*).

Rotational state-resolved differential cross sections (DCS) for the j-changing collisions of HCl by Ar are presented. A new crossed-molecular beam velocity-mapped imaging apparatus is used to measure the full (θ=0-180°) DCS for $j=0 \rightarrow j'=1,2,..,6$ rotational energy transfer at a center-of-mass energy of about 538 cm^{-1}. The j=0 state accounts for over 97% of the initial HCl rotational state population, and the scattering products are state-selectively ionized via (2+1) REMPI through the E-state, allowing for the direct extraction of state-to-state DCSs in the center-of-mass frame. The angular distributions for the experimental DCSs become increasingly backscattered as Δj increases, but do so non-monotonically, as $j'=3$ is more forward scattered than $j'=2$. Images for the even Δjs $0 \rightarrow 2$ and $0 \rightarrow 4$ are similar, and those for the odd Δjs $0 \rightarrow 1$ and $0 \rightarrow 3$ also have similarities. The calculated cross sections, based upon the HCl-Ar H6(4,3,0) potential of Hutson [*J. Phys. Chem.* 96, 4237-4247 (1992)], agree qualitatively with the experimental cross sections. However, there are significant differences between the theoretical and experimental results, where many of the principle features in the calculated DCSs lie 10-30° more back scattered than the same features in the experimental DCSs. These results may suggest that an adjustment to the repulsive region of the H6(4,3,0) potential is required.

TECHNICAL MEETINGS

(Current Additions to this List are Indicated by a Diamond Bullet Marking)

MARCH 5-8, 2000

8th INTERNATIONAL CONFERENCE ON NUMERICAL COMBUSTION
Amelia Island FL.

Conference Topics Include:

- Turbulence
- Kinetics
- Detonation
- Flames
- Pollution
- Microgravity
- Ignition
- Applications of Parallel Processing
- Tera-scale Computation of Combustion Applications
- Material Synthesis
- Droplets and Sprays
- Heterogeneous Combustion
- Energetic Materials (Propellants and Explosives)
- Engine and Furnace Combustion
- Fires
- Adaptive Numerical Methods
- Software Engineering for Combustion Applications

Invited Speakers Include:

- Premixed Turbulent Combustion: DNS into Modeling, R. Stewart Cant, University of Cambridge, United Kingdom
- Numerical Modeling of Combustion Control in Ramjets, Sergei Frolov, Semenov Institue of Chemical Physics, Russia
- Aerothermochemistry of Flames, Peter Lindstedt, Imperial College, United Kingdom
- Experimental Measurements of Solid Propellant Flame Structure for Model Validation, Timothy Parr, U.S. Naval Air Warfare Center
- Some New Developments in Pre-Mixed Gaseous Combustion, Gregory I. Sivashinsky, Tel Aviv University, Israel
- The Impact of the Accelerated Strategic Computing Initiative on Numerical Combustion, Charles K. Westbrook Lawrence Livermore National Laboratory

Information: Society for Industrial and Applied Mathematics, 3600 University Science Center, Philadelphia, PA 19104, http://www.siam.org/meetings/

MARCH 5-9, 2000

2000 SPRING NATIONAL MEETING OF THE AMERICAN INSTITUTE OF CHEMICAL ENGINEERS ON ADVANCED NEW TECHNOLOGIES IN INDUSTRY
Atlanta GA.

Topics will Include:

- 12th Ethylene Producers Conference
- 34th Loss Prevention Conference

- 4th International Conference on Microreaction Technology
- 3rd International Conference on Refining Processes

Information: W.S. Winston Ho, Meeting Program Chair, Department of Chemical and Materials Engineering, 177 Anderson Hall, Lexington, KY 40506, (606) 257-4815, Fax (606) 323-1929, e-mail: wsho@engr.uky.edu

MARCH 6-9, 2000

SAE INTERNATIONAL CONGRESS AND EXPOSITION
Detroit MI.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

MARCH 6-9, 2000

25th INTERNATIONAL TECHNICAL CONFERENCE ON COAL UTILIZATION AND FUEL SYSTEMS
Clearwater FL.

Information: B. Sakkestad, Coal Utilization and Fuel Systems Conference Committee, 104 Edith Drive, Rockville, MD 20850, (301) 294-6080, Fax (301) 294-7480, e-mail: barbarasak@aol.com, web: coaltechnologies.com

MARCH 9-11, 2000

JOINT SPRING MEETING OF THE TEXAS SECTIONS OF THE APS, AAPT AND ZONE 13 OF THE SPS
College Station TX.

Information: R.B. Clark, Department of Physics, Texas A&M University, College Station, TX 77843, (409) 845-3332, Fax (409) 845-2590, e-mail: rbc@tamu.edu, http://www.aps.org/meet/TSS00/

MARCH 12-14, 2000

ASTM COMMITTEE E-13 ON MOLECULAR SPECTROSCOPY
New Orleans LA.

Information: G. Collins, ASTM, (610) 832-9715, Fax (610) 832-9635, e-mail: gcollins@astm.org, http://www.astm.org

MARCH 12-17, 2000

THE PITTSBURGH CONFERENCE, PITTCON 2000
New Orleans LA.

Information: The Pittsburgh Conference, 300 Penn Center Boulevard, Suite 332, Pittsburgh, PA 15235, (412) 825-3220, Fax (412) 825-3224, e-mail: pittconinfo@pittcon.org, http://www.pittcon.org/

MARCH 13-14, 2000

SPRING MEETING OF THE WESTERN STATES SECTION OF THE COMBUSTION INSTITUTE
Colorado School of Mines, Golden CO.

Information: W.J. Pitz, L-353, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94551, (925) 422-7730, Fax (925) 422-2644, e-mail: pitz@llnl.gov, http://www.wssci.org/

MARCH 13-14, 2000

DATA FOR SCIENCE AND SOCIETY: 2nd NATIONAL CONFERENCE ON SCIENTIFIC AND TECHNICAL DATA
Washington DC.

Information: P.F. Uhlir, Director, U.S. National Committee for CODATA, National Research Council, Rm. 242, 2101 Constitution Avenue, NW, Washington, DC 20418, (202) 334-2688, Fax (202) 334-2139, e-mail: codataco@nas.edu, http://www.nationalacademies.org/usnc-codata

MARCH 20-24, 2000

MARCH MEETING OF THE AMERICAN PHYSICAL SOCIETY
Minneapolis MN.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

MARCH 26-30, 2000

SPRING NATIONAL MEETING OF THE AMERICAN INSTITUTE OF CHEMICAL ENGINEERS
Atlanta GA.

Information: Meetings Department, American Institute of Chemical Engineers, United Engineering Center, 345 East 47th Street, New York, NY 10017, (212) 2705-7338 or (800) 242-4363, http://www.aiche.org

MARCH 26-31, 2000

219th NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
San Francisco CA.

Division of Analytical Chemistry:

- New Frontiers in Analytical Chemistry
- Analytical Problems of the 21st Century
- Limitations of Present Analytical Tools
  T.R. Williams, College of Wooster, Wooster, OH 44691, (330) 263-2115, e-mail: williams@acs.wooster.edu

Division of Fuel Science:

- Fuel Science in the Year 2000: Where Do We Stand, Where Do We Go From Here?
  G.P. Huffman, 533 S. Limestone Street, Suite 111, University of Kentucky, Lexington, KY 40506-0043, (606) 257-4027, Fax (606) 257-7215 e-mail: cffls@pop.uky.edu

- Advances in F-T Chemistry
  B.H. Davis, Center for Applied Energy Research, University of Kentucky, Lexington, KY 40511, (606) 257-0251, Fax (606) 257-0302, e-mail: davis@alpha.caer.uky.edu
- Molecular Modeling of Solid-Fuel Reactions
  L.R. Radovic, Fuel Science Program, Pennsylvania State University, 217 Academic Projects Building, University Park, PA 16802, (814) 863-0594, Fax (814) 865-3075, e-mail: lrr3@psu.edu
- Applications of X-ray and Gamma Ray Techniques in Fuel Science
  K.A. Carrado, CHM/200, 9700 S. Cass Avenue, Argonne National Laboratory, Argonne, IL 60439-4831, (630) 252-7968, Fax (630) 252-9288, e-mail: kcarrado@anl.gov
- Particulate Matter and Fossil Fuel Combustion
  T.J. Feeley III, Department of Energy, Federal Energy Technology Center, P.O. Box 10940, Pittsburgh, PA 15236, (412) 892-6134, Fax (412) 892-5914, e-mail: feeley@fetc.doe.gov
- Solid Fuel Chemistry
  F. Huggins, South Limestone Street, Suite 111, University of Kentucky, Lexington, KY 40506, (606) 257-4045, Fax (606) 257-7215, e-mail: fhuggins@engr.uky.edu

Division of Petroleum Chemistry:
- New Chemistry of Fuel Additives
  D. Daly, Fuel Products, Strategic Technology, Lubrizol Co., 29400 Lakeland Blvd., Wickliffe, OH 44092, (440) 943-1200 ext. 4261, Fax (440) 943-9022, e-mail: dtd@lubrizol.com
- CO_2 Conversion and Utilization in Refinery and Chemical Processing
  C. Song, Pennsylvania State University, 209 Academic Projects Building, University Park, PA 16802, (814) 863-4466, Fax (814) 865-3075, e-mail: csong@psu.edu; A.M. Gaffney, DuPont Central R&D, Experimental Station, P.O. Box 80262, Wilmington, DE 19880, (302) 695-1800, Fax (302) 695-8347, e-mail: anne.m.gaffney@usa.dupont.com

Division of Physical Chemistry:
- Physical Chemistry at High Pressure and Temperature
  A.P. Alivisatos, Department of Chemistry, University of California, Berkeley CA 94720, (510) 643-7371, Fax (510) 642-6911, e-mail: alivis@uclink4.berkeley.edu; R. Jeanloz, Department of Geology & Geophysics, University of California, Berkeley CA 94720, (510) 642-2639, Fax (510) 643-9980, e-mail: jeanloz@uclink.berkeley.edu
- Atmospheric Chemistry (Harold Johnston Festschrift)
  C.E. Miller, Department of Chemistry, Haverford College, Haverford, PA 19041, (610) 896-1388, Fax (610) 896-4904, e-mail: cmiller@haverford.edu
- Potential Energy Surfaces: From Polyatomics to Macromolecules
  L.X. Dang, EMSL, Pacific Northwest National Laboratory, P.O. Box 999, Richland, WA 99352, (509) 375-2034, Fax (509) 375-6631, lx_dang@pnl.gov

Information: From the Individual Chairpersons or from Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

Deadline: 4 Copies of 150-Word Abstract (Original on ACS Abstract Form to Symposium Organizer by November 1, 1999 (Analytical and Physical Chemistry), October 15, 1999 (Fuel and Petroleum Chemistry).

MARCH 26-31, 2000

CORROSION/2000
Orlando FL.

Information: NACE Headquarters, Meetings Department, P.O. Box 218340, Houston, TX 77218, (281) 228-6200, Fax (281) 228-6300, http://www.nace.org

APRIL 3-5, 2000

ROYAL SOCIETY OF CHEMISTRY FARADAY DISCUSSION ON MOLECULAR PHOTOIONIZATION
York UK.

Information: K. Muller-Dethlefs, Department of Chemistry, The University of York, Heslington, York YO10 5DD, UK, 44(0) 1904 434526, Fax 44(0) 1904 434527, e-mail: KMD6@York.ac.uk, http://www.rsc.org/pdf/confs/fara115.pdf

APRIL 3-6, 2000

3rd INTERNATIONAL SYMPOSIUM ON TURBULENCE, HEAT AND MASS TRANSFER
Nagoya, Japan.

Information: T. Tsuji, Symposium Secretary, Department of Mechanical Engineering, Nagoya Institute of Technology, Gokiso-cho, Showa-ku, Nagoya 466-8555, Japan, (81) 52-735-5333, Fax (81) 52-735-5359, e-mail: tsuji@heat.mech.nitech.ac.jp, http://heat.mech.nitech.ac.jp/thmt3/

APRIL 3-6, 2000

41st AIAA/ASME/ASCE/AHS/ASC STRUCTURES, STRUCTURAL DYNAMICS AND MATERIALS CONFERENCE
Atlanta GA.

Information: M. Kamat, School of Aerospace Engineering, Georgia Institute of Technology, Atlanta, GA 30332, (404) 894-7439, Fax (404) 894-9313, e-mail: manohar.kamat @aerospace.gatech.edu, or the respective professional society webpages.

APRIL 4-10, 2000

10th INTERNATIONAL CONFERENCE ON HIGH TEMPERATURE MATERIALS CHEMISTRY
Aachen, Germany.

Information: Klaus Hilpert, Forschungszentrum Julich GmbH, Institut fur Werkstoffe der Energietechnik, Julich, Germany D-52425, (49) 2461 613280, Fax (49) 2461 613699, e-mail: k.hilpert@fz-juelich.de

APRIL 7-8, 2000

NEW YORK SECTION SPRING MEETING OF THE AMERICAN PHYSICAL SOCIETY
Corning NY.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

APRIL 8-12, 2000

SPRING TECHNICAL CONFERENCE OF THE ASME INTERNAL COMBUSTION ENGINE DIVISION
San Antonio TX.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7054, Fax (212) 705-7143, http://www.asme.org

APRIL 10-11, 2000

SPIE'S REGIONAL MEETING ON OPTOELECTRONICS, PHOTONICS AND IMAGING: OPTO SOUTHWEST
Albuquerque NM.

Information: B. Peterson, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: bonnie@spie.org, www.spie.org/info/sw/

APRIL 10-14, 2000

10th INTERNATIONAL IUPAC CONFERENCE ON HIGH TEMPERATURE MATERIALS CHEMISTRY
Aachen, Germany.

Topics will Include:
- Synthesis, Properties, and Application of High Temperature Materials
- Vaporization, Molecules, and Clusters
- Interface Processes (Corrosion, Oxidation, Diffusion)
- Technical Processes and Devices at High Temperatures
- Thermodynamic and Kinetic Measurements, Modeling and Databases

Information: K. Hilpert, Forschungszentrum Julich GmbH, Institut fur Werkstoffe der Energietechnick (IWE 1), 52425 Julich, Germany, (49) 2461 61 3280, Fax (49) 2461 61 3699, e-mail: k.hilpert@fz-juelich.de, http://www.fz-juelich.de/oea/termine.html

APRIL 10-14, 2000

3rd INTERNATIONAL SEMINAR IN FIRE AND EXPLOSION HAZARDS
Lake Windermere, UK.

Information: G. Makhviladze, Centre for Research in Fire and Explosion Studies, University of Central Lancashire, Preston PR1 2HE, UK, (01772) 893222, Fax (01772) 892916, e-mail: g.makhviladze@uclan.ac.uk, http://www.uclan.ac.uk/commerc/fire.htm

APRIL 11-13, 2000

GASIFICATION FOR THE FUTURE
Noordwijk, The Netherlands.

Information: J. Black, IChemE's Conference Department, 165-189 Railway Terrace, Rugby, Warwickshire CV21 3HQ, UK, (44) 1788-578214, Fax (44) 1788-577182, e-mail: jblack@icheme.org.uk

APRIL 11-14, 2000

5th EUROPEAN CONFERENCE ON INDUSTRIAL FURNACES AND BOILERS
Porto, Portugal.

Information: INFUB c/o Albino Reis, Rua Gago Coutino, 185-187, 4435 Rio Tinto, Portugal, (2) 9734624/9730747, Fax (2) 9730746, e-mail: conference@infub.pt, http://www.infub.pt

APRIL 12-14, 2000

3C STEREO AND HOLOGRAPHIC PIV APPLICATION TO TURBULENCE MEASUREMENTS: EUROMECH COLLOQUIUM 411
Rouen, France.

Information: M. Trinite, CORIA-UMR 6614, Universite et INSA de Rouen, F-76821 Mont Saint Aignan Cedex, France, (33) 2-35-14-65-58, Fax (33) 2-35-70-83-84, e-mail: trinite@coria.fr

APRIL 14-15, 2000

NEW ENGLAND SECTION SPRING MEETING OF THE AMERICAN PHYSICAL SOCIETY
Providence RI.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

APRIL 16-18, 2000

SPRING TECHNICAL MEETING OF THE CENTRAL STATES SECTION OF THE COMBUSTION INSTITUTE
Indianapolis IN.

Invited Papers Include:

- The Real Sequence of Processes to be Modeled in Diesel Engine Combustion
  P.F. Flynn, Cummins Engine Co., Inc.
- A Current Perspective on In-Cylinder Turbulent Thermal-Fluids Processes in Spark Ignited Reciprocating IC Engines
  D. Haworth, Pennsylvania State University
- Multidimensional Modeling of Reacting Flow in Stationary Combustors
  W.A. Fiveland, Combustion Engineering, Inc.
- Modeling of Gas-Turbine Combustors
  M.S. Anand, Rolls Royce Allison

Information: D.L. Reuss, General Motors R&D, 30500 Mound Road, Warren, MI 48090, (810) 986-0887, Fax (810) 986-0176, e-mail: dreuss@gmr.com
Deadline: Submit Abstract by January 4, 2000, 6-Page Paper by March 1, 2000. Abstracts of Poster Presentations by February 15, 2000.

APRIL 24-28, 2000

MATERIALS RESEARCH SOCIETY SPRING MEETING
San Francisco CA.

Information: Materials Research Society, Meetings Department, 506 Keystone Drive, Warrendale, PA 15086, (412) 779-3003, e-mail: info@mrs.org

APRIL 26-30, 2000

2nd INTERNATIONAL CONFERENCE ON ATOMIC AND MOLECULAR DATA AND THEIR APPLICATIONS
Oxford UK.

Information: K. Berrington, e-mail: k.berrington@shu.ac.uk, http://physics.nist.gov/icamdata

APRIL 29-MAY 1, 2000

ANNUAL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Long Beach CA.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

MAY 2-4, 2000

HALON OPTIONS TECHNICAL WORKING CONFERENCE
Albuquerque NM.

Information: L. Oliver, The University of New Mexico, 901 University Boulevard SE, Albuquerque, NM 87106, (505) 272-7250, Fax (505) 272-7203, e-mail: oliver@nmeri.unm.edu

MAY 7-12, 2000

CLEO/QELS 2000
San Francisco CA.

Information: Meetings Department, American Physical Society, One Physics Ellipse, College Park, MD 20740, (301) 209-3286, http://www.osa.org/mtg_conf, http://physics.wm.edu/~cooke/dis/dis.html

MAY 8-11, 2000

ASME TURBO EXPO: LAND, SEA AND AIR
Munich, Germany.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (404) 847-0072 or (212) 591-7008, Fax (212) 705-7143, http://www.asme.org

MAY 8-11, 2000

UNITED ENGINEERING CONFERENCE ON THE EFFECTS OF COAL QUALITY ON POWER PLANT PERFORMANCE: ASH PROBLEMS, MANAGEMENT AND SOLUTIONS
Park City UT.

Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441, e-mail: engfnd@aol.com, http://www.engfnd.org/engfnd/conf.html

MAY 8-12, 2000

INTERNATIONAL CONFERENCE ON INCINERATION AND THERMAL TREATMENT TECHNOLOGIES
Portland OR.

Information: L.B. Cohen, University of California, EH&S, 300 University Tower, Irvine CA 92697, (949) 824-5859, Fax (949) 824-1900, e-mail: lbarnow@uci.edu

MAY 9-11, 2000

5th INTERNATIONAL CONFERENCE ON COAL UTILIZATION SCIENCE AND TECHNOLOGY
Budapest, Hungary.

Information: Z. Katona, Department of Energy, Technical University of Budapest, 1111 Budapest, Muegyetem rkp. 3, Hungary, Fax (1) 463-3273, or in the UK, J. Tucker, 44(0) 1242-763361.

MAY 14-19, 2000

197th MEETING OF THE ELECTROCHEMICAL SOCIETY
Toronto, Ontario, Canada.

Topics Include:
- General Session on Corrosion
- Plasma Processing
- 15th International Conference on Chemical Vapor Deposition
- Sensors for Energy Technologies

Information: http://www.electrochem.org/meetings

MAY 16-19, 2000

33rd MIDDLE ATLANTIC REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Newark DE.

Information: G.L. Trainor, DuPont Pharmaceuticals Co., P.O. Box 80353, Wilmington, DE 19880, (302) 695-3580, Fax (302) 695-8344, e-mail: trainogl@carbon.dmpc.com

MAY 17-18, 2000

CONFERENCE ON SELECTIVE CATALYTIC AND NONCATALYTIC REDUCTION FOR NO_x CONTROL
Pittsburgh PA.

Information: K. Lockhart, FETC Conference Services, 626 Cochrans Mill Road, P.O. Box 10940, MS 922-178C, Pittsburgh, PA 15236, (412) 386-4763, Fax (412) 386-6486, e-mail: lockhart@fetc.doe.gov

MAY 17-19, 2000

32nd Central Regional Meeting of the American Chemical Society
Covington KY.

Information: R. D'Alonzo, Procter & Gamble, Sharon Woods Technical Center, 11450 Grooms Road, Cincinnati, OH 45242, (513) 626-1977, Fax (513) 626-5145, e-mail: dalonzorp@pg.com

MAY 19-20, 2000

Northwest Section Meeting of the American Physical Society
Eugene OR.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

MAY 22-26, 2000

4th Minsk International Heat and Mass Transfer Forum
Minsk, Belarus.

Information: I. Gurevich, Secretary of the MIF-IV Organizing Committee, A.V. Luikov Heat and Mass Transfer Institute, National Academy of Sciences of Belarus, 15, P. Brovka St., Minsk, 220072, Belarus, (375) 17.284-21-36, Fax (375) 17.232-25-13, e-mail: igur@hmti.ac.by, http://www.itmo.by/forum/forum7/index.html

JUNE 4-7, 2000

32nd Great Lakes Regional Meeting of the American Chemical Society
Fargo ND.

Information: G.J. McCarthy, North Dakota State University, Department of Chemistry, Ladd Hall 104B, Fargo, ND 58105, (701) 231-7193, Fax (701) 231-8883, e-mail: gmccarth@prarie.nodak.edu

JUNE 4-8, 2000

Turn of the Century in Atomic Spectrometry and Element Analysis: Past, Present and Future
Interlaken, Switzerland.

Information: G. Vujicic, SASP c/o IWM, Industriestr. 59, Glattbrugg, Switzerland CH-8152, (41) (0) 1 810 57 72, Fax (41) (0) 1 810 09 78, e-mail: gvujicic@swissonline.ch, http://www.sasp.ch/

JUNE 8-10, 2000

Joint 55th Northwest/16th Rocky Mountain Regional Meeting of the American Chemical Society
Idaho Falls ID.

Information: E.G. Meyer, 214 Arts & Sciences, University of Wyoming, Laramie, WY 82071, (307) 766-5445.

JUNE 11-12, 2000

16th World Petroleum Congress
Calgary, Alberta, Canada

Information: 16th World Petroleum Congress, 1350, 144-4 Avenue SW, Calgary, Alberta, Canada T2P 3N4, (403) 218-2000, Fax (403) 218-2002, e-mail: cdn.assoc@wpc2000.com, web: www.wpc2000.com

JUNE 11-14, 2000

ASME/ZSITS International Thermal Science Seminar
Bled, Slovenia.

Information: I. Golobic, Faculty of Mechanical Engineering, University of Ljubljana, Askerceva 6, 1000 Ljubljana, Slovenia, (386) 61-1771420, Fax (386) 61-218567, e-mail: iztok.golobic@uni-lj.si, or A.E. Bergles, 180 River View Lane, Centerville, MA 02632, Phone/Fax (508) 790-4873, e-mail: abergles@aol.com, http://www.ltt.uni-lj.si/itss2000/

JUNE 11-15, 2000

Summer Meeting of the ASME Fluids Engineering Division
Boston MA.

Symposia will Include:

- Flows in Manufacturing Processes
- Numerical Developments in CFD
- Non-Invasive Measurements in Multiphase Flow
- Advances in Numerical Modeling of Aerodynamics and Hydrodynamics in Turbomachinery
- Erosion Processes
- Fluid Flow in Microsystems: Measurement, Analysis, and Applications
- Numerical Methods for Multiphase Flows
- Experimental and Numerical Flow Visualization and Laser Anemometry

Forums will be Held on the Following Topics:

- Finite Element Applications in Fluid Dynamics
- Turbulent Flows
- Laminar Flows
- High Speed Jet Flows
- Advances in Fluids Engineering Education
- CFD Applications in Automotive Flows
- Bifurcation, Instability, and Hysteresis in Fluid Flow
- Three-Dimensional Flows
- CFD Applications in Large Facilities
- Open Forum on Multiphase Flows
- Submicron Particle Flows
- Fluid Measurements and Instrumentation
- Fluid Machinery Forum
- Advances in Free Surface and Interface Fluid Dynamics
- Simulation of the Interaction of Transportation Vehicles with the Environment
- Forum on Developments in CFD Code Verification and Validation
- Cavitation and Multiphase Flow Forum

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 705-7037, Fax (212) 705-7143, http://www.asme.org

JUNE 11-15, 2000

48th ASMS CONFERENCE ON MASS SPECTROMETRY AND ALLIED TOPICS
Long Beach CA.

Information: http://www.asms.org

JUNE 12-16, 2000

55th SYMPOSIUM ON MOLECULAR SPECTROSCOPY
Columbus OH.

Information: T.A. Miller, International Symposium on Molecular Spectroscopy, Department of Chemistry, The Ohio State University, 120 West 18th Avenue, Columbus, OH 43210.

JUNE 14-17, 2000

DIVISION OF ATOMIC, MOLECULAR AND OPTICAL PHYSICS OF THE AMERICAN PHYSICAL SOCIETY
Storrs CT.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

JUNE 15-17, 2000

JOINT 55th ACS NORTHWEST/16th ROCKY MOUNTAIN REGIONAL MEETING
Idaho Falls ID.

Information: E.G. Meyer or D. Nelson, 214 Arts & Sciences, University of Wyoming, Laramie, WY 82071, (307) 766-5445, Fax (307) 766-2697, e-mail: egmeyer@uwyo.edu or danelson@wyoming.com; T. Allen or F. Stewart, INEEL, P.O. Box 1625, MS 2008, Idaho Falls, ID 83415, (208) 526-8594, Fax (208) 526-8541, e-mail: fsf@inel.gov, web site: http:/www2.ida.net/acsid/norm2000/

JUNE 18-21, 2000

29th NORTHEAST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Storrs CT.

Information: G. Epling, University of Connecticut, 215 Glenbrook Road, Storrs, CT 06269, (860) 486-3214, Fax (860) 486-2981, e-mail: epling@nucleus.chem.uconn.edu

JUNE 18-22, 2000

ANNUAL MEETING OF THE AIR AND WASTE MANAGEMENT ASSOCIATION
Salt Lake City UT.

Information: Air and Waste Management Association, Member Services, One Gateway Center, Third Floor, Pittsburgh, PA 15222, (800) 270-3444 or (412) 232-3444, Fax (412) 232-3450, http://www.awma.org

JUNE 18-23, 2000

OPTICS IN COMPUTING
Quebec City, Quebec, Canada.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

JUNE 19-20, 2000

CEC/SAE FUELS AND LUBRICANTS SPRING MEETING AND EXPOSITION
Le Palais des Congress, Paris, France.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, http://www.sae.org

JUNE 19-22, 2000

21st AIAA ADVANCED MEASUREMENT TECHNOLOGY AND GROUND TESTING CONFERENCE: FLUIDS 2000 AND EXHIBIT: 31st AIAA PLASMADYNAMICS AND LASERS CONFERENCE: 34th AIAA THERMOPHYSICS CONFERENCE
Denver CO.

Information: J.A. Morrow, Department of Aeronautics, United States Air Force Academy, 2354 Fairchild Drive, #6H22, U.S. Air Force Academy, CO 80840, (719) 333-3434, Fax (719) 333-4813, e-mail: MorrowJA.dfan@usafa.af.mil, or http://www.aiaa.org

JUNE 21-23, 2000

60th PHYSICAL ELECTRONICS CONFERENCE
Baton Rouge LA.

Information: R.L. Kurtz, Department of Physics and Astronomy, 202 Nicholson Hall, Louisiana State University, Baton Rouge, LA 70803, (225) 388-4028, Fax (225) 388-5855, http://www.physicalelectronics.org/

♦ JUNE 26-28, 2000

HEAT TRANSFER 2000: 6th INTERNATIONAL CONFERENCE ON ADVANCED COMPUTATIONAL METHODS
Madrid, Spain.

Information: e-mail: shanley@wessex.ac.uk, http://www.wessex.ac.uk/conferences/2000/heat2000

JUNE 26-30, 2000

INTERNATIONAL WORKSHOP ON UNSTEADY COMBUSTION AND INTERIOR BALLISTICS
St. Petersburg, Russia.

Information: V. Babuk, e-mail: kaf-m1@bstu.spb.su, or babuk@peterlink.ru

♦ JUNE 27-30, 2000

EUROMECH 8th EUROPEAN TURBULENCE CONFERENCE
Barcelona, Spain.

Information: ETC8 Secretariat, International Center for Numerical Methods in Engineering (CIMNE), C1 Campus Nord, Universita Politecnica de Catalunya, Barcelona E-08034, Spain, (34) 932057016, Fax (34) 9340 16517, e-mail: leia@cimne.upc.es, http://www.icimne.upc.es/etc8.html

JULY 1-7, 2000

WORLDWIDE RENEWABLE ENERGY CONGRESS
Brighton UK.

Information: A. Sayrigh, 147 Hilmanton, Lower Earley, Reading RG6 4HN, UK.

♦ JULY 2-6, 2000

FTEC 2000: INTERNATIONAL CONFERENCE ON FLUID AND THERMAL ENERGY CONVERSION
Jakarta, Indonesia.

Information: A. Suwono, Thermodynamics Laboratory, Inter University Research Center for Engineering Sciences, Institute of Technology of Bandung, Jalan Tamansari 126, Bandung 40132, Indonesia, (62) 22-250-2342, Fax (62) 22-250-2342, e-mail: ari@termo.pauir.itb.ac.id, or ftec2000@ibm.net, http://www.pauir.itb.ac.id/FTEC2000

♦ JULY 3-6, 2000

7th AUSTRALASIAN HEAT AND MASS TRANSFER CONFERENCE
Townsville, Queensland, Australia.

Information: J. Patterson, Chair, Gary Brassington, Secretary, James Cook University, Townsville, Queensland, Australia, (61) 7-4781-4346, Fax (61) 7-4775-1184, e-mail: 7ahmtc@jcu.edu.au, http://www.eng.jcu.edu.au/AHMTC/

JULY 9-14, 2000

6th POLISH CONFERENCE ON ANALYTICAL CHEMISTRY
Gliwice, Poland.

Information: 6th Polish Conference on Analytical Chemistry, Department of Analytical and General Chemistry, Silesian Technical University, ul. M. Strzody 9, 44-100 Gliwice, Poland, phone/fax 48-32-237-12-05, e-mail: analityk@zeus.polsl.gliwice.pl, http://www.polsl.gliwice.pl/~analityk

JULY 10-13, 2000

10th International Symposium on Applications of Laser Techniques to Fluid Mechanics
Lisbon, Portugal.

Information: M.V. Heitor, Department of Mechanical Engineering, Instituto Superior Tecnico, Av. Rovisco Pais, 1049-001 Lisboa, Portugal, (351) 1-841-7379/7732, Fax (351) 1-849-6156, e-mail: llaser@in3dem.ist.utl.pt, http://in3.dem.ist.utl.pt/lisboa-laser

JULY 16-19, 2000

36th AIAA/ASME/SAE/ASEE Joint Propulsion Conference and Exhibit on Propulsion: The Key to Exploring New Worlds
Huntsville AL.

Information: B. Noblitt, Conference General Chair, TRW, Suite 1231, 303 Williams Avenue, Huntsville, AL 35801, (256) 533-3714, Fax (256) 533-0137, e-mail: bobby.noblitt@trw.com, or http://www.aiaa.org/calendar

JULY 16-20, 2000

8th International Conference on Liquid Atomization and Spray Systems
Pasadena CA.

Information: D. Talley, USAF Research Laboratory, AFRL/PRSA, 10 East Saturn Boulevard, Edwards AFB, CA 93524, (661) 275-6174, Fax (661) 275-6245, e-mail: douglas_talley@ple.af.mil, http://www.iclass2000.uci.edu/

JULY 17-20, 2000

10th Biennial National Atomic Spectroscopy Symposium of the Royal Society of Chemistry
Sheffield, UK.

Information: P. Krause, Centre for Analytical Science, Dainton Building, Brookhill, Sheffield, S3 7HF, UK, 44(0) 114-222-3652, Fax 44(0) 114-222-3650, e-mail: p.krause@sheffield.ac.uk, http://www.rsc.org/lap/rsccom/dab/ana002.htm

JULY 22-27, 2000

18th Symposium on Photochemistry: Photochemistry into the New Century
Dresden, Germany.

Information: S.E. Braslavsky, Max-Planck Institut fur Strahlenchemie, Postfach 101365, D-45413 Mulheim an der Ruhr, Germany, (49) 208-306-3681, Fax (49) 208-306-3951, e-mail: braslavskys@mpi-muelheim.mpg.de, http://www.chm.tu-dresden.de/photo/iupac2000/

JULY 23-26, 2000

ASME INTERNATIONAL JOINT POWER GENERATION CONFERENCE AND EXPOSITION
Miami Beach FL.

Information: N.A. Moussa, BlazeTech Corporation, 24 Thorndike Street, Cambridge, MA 02141, (617) 661-0700, Fax (617) 661-9242, amoussa@blazetech.com, or http://www.asme.org/conf/

JULY 23-27, 2000

16th INTERNATIONAL SYMPOSIUM ON GAS KINETICS
Cambridge UK.

Information: G. Southwell, Secretary to the 16th International Symposium on Gas Kinetics, University Chemical Laboratory, Lensfield Road, Cambridge, CB2 1EW, England, Fax (1223) 336362, http://www.gk2.ch.cam.ac.uk

JULY 23-28, 2000

ENERGEX 2000: 8th INTERNATIONAL ENERGY FORUM
Las Vegas NV.

Topics will Include:
- Renewable Energies
- Clean Coal Technologies
- Fossil Fuels
- Energy and Economics
- Climatic Change
- International Law
- General Topics
- International Reports
- Nuclear Energy
- Architecture

Information: P. Catania, Faculty of Engineering, University of Regina, Regina, SK S4S 0A2, Canada, (306) 585-4363, Fax (306) 585-4855, e-mail: peter.catania@uregina.ca, http://www2.regina.ism.ca/ief/index/htm or http://www.energysource.com/ief/updates/

♦ JULY 24-26, 2000

AIR POLLUTION 2000: 8th INTERNATIONAL CONFERENCE ON MODELING, MONITORING AND MANAGEMENT OF AIR POLLUTION
Cambridge, UK.

Information: S. Walsh, Conference Secretariat, Air Pollution 2000, Wessex Institute of Technology, Ashurst Lodge, Ashurst, Southampton SO4O 7AA, UK, (44) 238-029-3223, Fax (44) 238-029-2853, e-mail: wit@wessex.ac.uk, http://www.wessex.ac.uk/conferences/2000/

♦ JULY 24-28, 2000

35th INTERSOCIETY ENERGY CONVERSION ENGINEERING CONFERENCE
Las Vegas NV.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7008, Fax (212) 705-7143, http://www.asme.org

JULY 30-AUGUST 4, 2000

SPIE ANNUAL MEETING
San Diego CA.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

JULY 30-AUGUST 4, 2000

28th INTERNATIONAL SYMPOSIUM ON COMBUSTION
Edinburgh, Scotland.

Information: S.S. Terpack, The Combustion Institute, 5001 Baum Boulevard, Suite 635, Pittsburgh, PA 15212, (412) 687-1366, Fax (412) 687-0340, e-mail: combust@telerama.lm.com

♦ JULY 30-AUGUST 4, 2000

GORDON RESEARCH CONFERENCE ON MOLECULAR ELECTRONIC SPECTROSCOPY AND DYNAMICS
New London NH.

Information: R.W. Field, Chair, Massachusetts Institute of Technology, rwfield@mit.edu; E. Bernstein, Vice-chair, Colorado State University, erb@lamar.colostate.edu; or J. Skinner, Chair, University of Wisconsin-Madison, skinner@chem.wisc.edu

AUGUST 6-11, 2000

15th INTERNATIONAL CONFERENCE ON NUCLEATION AND ATMOSPHERIC AEROSOLS
Rolla MO.

Information: B. Hale, University of Missouri, 205 Physics, Rolla, MO 65409, (573) 341-4795, e-mail: bhale@umr.edu or marrku.kulmala@helsinki.fi, http://www.umr.edu/~icnaa

AUGUST 6-11, 2000

16th IUPAC CONFERENCE ON CHEMICAL THERMODYNAMICS
Halifax, Nova Scotia, Canada.

Information: M.A. White, Department of Chemistry, Dalhousie University, Halifax, Nova Scotia B3H 4J3, Canada, (902) 494-3894, Fax (902) 494-1310, e-mail: mary.anne.white@dal.ca, http://IS.DAL.CA/~ICCT

AUGUST 8-12, 2000

8th INTERNATIONAL CONFERENCE ON ELECTRONIC SPECTROSCOPY AND STRUCTURE
Berkeley CA.

Information: ICESS8, Advanced Light Source, Lawrence Berkeley National Laboratory, MS 6-2100, Berkeley, CA 94720, Fax (510) 486-4773, e-mail: icess@lbl.gov, http://www-als.lbl.gov/icess

AUGUST 13-16, 2000

5th INTERNATIONAL CONFERENCE ON GREENHOUSE GAS TECHNOLOGIES
Cairns, Queensland, Australia.

Information: GHGT-5 Secretariat, C. Paulson, CSIRO Energy Technology, PO Box 136, North Ryde, NSW 1670, Australia, (2) 9490-8790, Fax (2) 9490-8819, e-mail: c.paulson@det.csiro.au

AUGUST 13-18, 2000

TURBINE 2000, INTERNATIONAL SYMPOSIUM ON HEAT TRANSFER IN GAS TURBINE SYSTEMS
Izmir, Turkey.

Information: R.J. Goldstein, Conference Chair, Department of Mechanical Engineering, University of Minnesota, Minneapolis, MN 55455, (612) 625-5552, Fax (612) 625-3434, e-mail: rjgumn@mailbox.mail.umn.edu, http://ichmt.me.metu.edu.tr
Deadline: Abstracts Due by February 29, 2000.

AUGUST 14-17, 2000

18th AIAA APPLIED AERODYNAMICS CONFERENCE
Denver CO.

Information: N.E. Suhs, Applied Aerodynamic Technical Program Chair, Naval Air Systems Command, Building 2187, Unit 5, Suite 1390A, 48110 Shaw Road, Patuxent River, MD 20670, (301) 342-0311, Fax (301) 342-8585, e-mail: suhsne@navair.navy.mil, or http://www.aiaa.org/calendar
Deadline: Abstract by January 3, 2000

AUGUST 14-18, 2000

12th INTERNATIONAL CONGRESS ON THERMAL ANALYSIS AND CALORIMETRY
Copenhagen, Denmark.

Information: O.T. Sorensen, Materials Research Department, Riso National Laboratory, DK-4000 Roskilde, Denmark, 45-4677-5800, Fax 45-4677-5758, e-mail: o.toft.sorensen@risoe.dk, http://www.risoe.dk/ictac

AUGUST 16-22, 2000

JAHN TELLER SYMPOSIUM
Boston MA.

Information: M. Kaplan, Simmons College and Boston University, (617) 521-2727, e-mail: kaplan@buphy.bu.edu, or G. Zimmerman, Boston University, (617) 353-2189, e-mail: goz@buphy.bu.edu

AUGUST 20-22, 2000

34th ASME NATIONAL HEAT TRANSFER CONFERENCE
Pittsburgh PA.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7795, Fax (212) 705-7143, http://www.asme.org

♦ AUGUST 20-24, 2000

220th NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Washington DC.

Division of Analytical Chemistry:
- Detection of Explosives, Pre- and Post-Blast
  R.Q. Thompson, Oberlin College, Department of Chemistry, 130 W. Lorain Street, Oberlin, OH 44074, (440)775-8305, Fax (440) 775-6682, e-mail: robert.q.thompson@oberlin.edu

Division of Fuel Chemistry:
- 1990 Clean Air Act Amendments: A 10-Year Assessment
  J.J. Helble, University of Connecticut, Department of Chemical Engineering, U-222, Storrs, CT 06269, (860) 486-4602, Fax (860) 486-2959, e-mail: helble@eng2.uconn.edu
- Inorganics in Fossil Fuels, Waste Materials, and Biomass: Characterization, Combustion Behavior, and Environmental Issues
  C.L. Senior, Physical Sciences, Inc., 20 New England Business Center, Andover, MA 01810, (978) 689-0003, Fax (978) 689-3232, e-mail: senior@psicorp.com
- Waste Material Recycling for Energy and Other Applications
  S.V. Pisupati, Fuel Science Program, Pennsylvania State University, 404 Academic Projects Building, University Park, PA 16802, (814) 865-0874, Fax (814) 863-8892, e-mail: sxp17@psu.edu
- Fossil Fuels and Global Climate/CO_2 Abatement
  R. Warzinski, USDOE/FETC, Box 10940, Building 83-324, Pittsburgh, PA 15236, (412) 892-5863, e-mail: warzinsk@fetc.doe.gov
- Production of Fuels and Chemicals from Synthesis Gas
  D.B. Dadyburjor, Department of Chemical Engineering, P.O. Box 6102, West Virginia University, Morgantown, WV 26506, (304) 293-2111 ext 2411, Fax (304) 293-4139, e-mail: dadyburjor@cemr.wvu.edu
- Solid Fuel Chemistry
- Chemistry of Liquid and Gaseous Fuels
  F. Huggins, South Limestone St., Suite 111, University of Kentucky, Lexington, KY 40506, (606) 257-4045, Fax (606) 257-7215, e-mail: fhuggins@engr.uky.edu
- CO_2 Capture, Utilization and Sequestration
  R.P. Warzinski, Department of Energy, Federal Energy Technology Center, P.O. Box 10940, Building 83-324, Pittsburg, PA 15236, (412) 386-5863, Fax (412) 386-4806, e-mail: warzinsk@fetc.doe.gov; R.M. Enick, University of Pittsburgh, Department of Chemical

Engineering, 323 Benedum Engineering Hall, Pittsburgh, PA 15261, (412) 624-9649, e-mail: enick@engrng.pitt.edu

- Solid Fuel Chemistry and
- Chemistry of Liquid and Gaseous Fuels
  F.E. Huggins, University of Kentucky, Chemical and Materials Engineering, 533 S. Limestone Street, 111 Whalen Building, Lexington, KY 40506, (606) 257-4045, Fax (606) 257-7215, e-mail: fhuggins@engr.uky.edu

Division of Petroleum Chemistry:

- Emission Control in Petroleum Processing
  P. O'Connor, U.S. Ozkan, Department of Chemical Engineering, Ohio State University, 140 W. 19th Avenue, Columbus, OH 43210, (614) 292-6623, Fax (614) 292-3769, e-mail: ozkan.1@osu.edu
- Structure of Jet Fuels VI
  W.E. Harrison, Department of the Air Force, WL/POSF, Building 490, Area B, 1790 Loop Road N., Wright-Patterson AFB, OH 45433, (937) 255-6601, Fax (937) 255-1125, e-mail: harriswe@wl.pafb.af.mil

Division of Physical Chemistry:

- Chemistry Under Extreme Conditions
  R. Morris, AFRL/VSBP, 29 Randolph Rd., Hanscom AFB, MA 01731, (781) 377-8758, Fax (781) 377-5088, e-mail: morris@plh.af.mil
- Very Low Temperature Spectroscopy and Dynamics
  W. Stwalley, Department of Physics, University of Connecticut, 2152 Hillside Road, Storrs, CT 06269, (860) 486-4924, Fax (860) 486-3346, e-mail: stwalley@uconnvm.uconn.edu
- Femtochemistry: Honoring Ahmed Zewail, the 1999 Chemistry Nobel Laureate
  M. Dantus, Department of Chemistry, Michigan State University, East Lansing, MI 48824-1322, (517) 355-9715, Fax (517) 353-1793, e-mail: dantus@msu.edu

Information: From the Individual Chairpersons or from the Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

AUGUST 20-25, 2000

17th INTERNATIONAL CONFERENCE ON RAMAN SPECTROSCOPY
Beijing, China.

Information: Shu-Lin Zhang, President of ICORS 2000, e-mail: icors@pku.edu.cn, http://icors.pku.edu.cn

AUGUST 22-25, 2000

9th INTERNATIONAL (MILLENNIUM) SYMPOSIUM ON FLOW VISUALIZATION
Edinburgh, Scotland.

Information: I. Grant, Heriot-Watt University, Edinburgh, Scotland, EH10 5PJ, UK, (44) 1314478800, Fax (44) 1314478660, e-mail: 9misfv@ode-web.demon.co.uk, Web Site: http://www.ode-web.demon.co.uk/9misfv
Deadline: Abstract Template should be Downloaded from the Web. 4 Pages or Less to be Submitted by December 12, 1999. Final Manuscripts Due May 15, 2000.

AUGUST 26-30, 2000

15th EUROPHYSICS CONFERENCE ON ATOMIC AND MOLECULAR PHYSICS OF IONIZED GASES
Miskolc-Lillafured, Hungary.

Information: Z. Donko, c/o Eotvos Lorand Physical Society, H-1371 Budapest, P.O. Box 433, Hungary, e-mail: escampig@elft.mtesz.hu, http://elft.mtesz.hu/escampig2000

AUGUST 27-31, 2000

14th INTERNATIONAL CONGRESS OF CHEMICAL AND PROCESS ENGINEERING
Prague, Czech Republic.

Information: CHISA 2000, Novotneho Lavka 5, 116 68 Praha 1, Czech Republic, (420) 2-2108-2333, Fax (420) 2-2108-2336, e-mail: chisa@csvts.cz, http://www.chisa.cz

AUGUST 27-SEPTEMBER 1, 2000

25th EUROPEAN CONGRESS ON MOLECULAR SPECTROSCOPY
Coimbra, Portugal.

Information: R. Fausto, Department of Chemistry, University of Coimbra, Coimbra, Portugal P-3049, (351) 39-852080, Fax (351) 39-827703, e-mail: rfausto@gemini.ci.uc.pt, http://qui.uc.pt/~rfausto/eucmos_xxv

AUGUST 27-SEPTEMBER 1, 2000

15th INTERNATIONAL MASS SPECTROMETRY CONFERENCE
Barcelona, Spain.

Information: Ana Costeja, Palau de Congressos, Departament de Convencions, Av. Reina Mª Cristina, s/n, 08004 Barcelona, Spain (34) 932-332-377, Fax (34) 934-262-845, e-mail: 15imsc@website.es, http://www.website.es/15imsc

SEPTEMBER 3-7, 2000

16th INTERNATIONAL CONFERENCE ON HIGH RESOLUTION MOLECULAR SPECTROSCOPY
Prague, Czech Republic.

Information: S. Urban, UFCH JH Academy of Sciences of the Czech Republic, Dolejskova 3, Prague, Czech Republic, CZ-18223, (420) 2-6605-3635, Fax (420) 2-858-2307, e-mail: praha2k@jh-inst.cas.cz, http://www.chem.uni-wuppertal.de/conference/

♦ SEPTEMBER 4-8, 2000

EUROPEAN AEROSOL CONFERENCE
Trinity College, Dublin, Ireland.

Information: The Aerosol Society, P.O. Box 34, Portishead, Bristol, BS20 7FE, UK, http://www.aerosol-soc.org.uk

SEPTEMBER 10-13, 2000

3rd EUROPEAN THERMAL SCIENCES CONFERENCE
Heidelberg, Germany.

Information: E. Hahne, Institut fur Thermodynamik und Warmetechnik, Pfaffenwaldring 6, 70550 Stuttgart, Germany, 49 (0) 711-685-3536, Fax 49 (0) 711-685-3503, e-mail: pm@itw.uni-stuttgart.de

SEPTEMBER 10-15, 2000

CONFERENCE ON LASERS AND ELECTRO-OPTICS (CLEO) AND THE INTERNATIONAL QUANTUM ELECTRONICS CONFERENCE (IQEC)
Nice, France.

Information: Optical Society of America, Meetings Department, 2010 Massachusetts Ave NW, Washington, DC 20036, (202) 223-0920, e-mail: confserv@osa.org

SEPTEMBER 10-15, 2000

1st INTERNATIONAL SYMPOSIUM ON MICROGRAVITY RESEARCH AND APPLICATION IN PHYSICAL SCIENCES AND BIOTECHNOLOGY
Sorrento, Italy.

Information: ESTEC, Conference Bureau, P.O. Box 299, 2200 AG Noordwijk, The Netherlands, (71) 5655005, Fax (71) 5655658, e-mail: confburo@estec.esa.nl

♦ SEPTEMBER 10-15, 2000

7th DURHAM CONFERENCE ON PLASMA SOURCE MASS SPECTROMETRY
Durham UK.

Information: G. Holland, Department of Geological Sciences, Science Laboratories, South Road, Durham City DH1 3LE, UK, e-mail: tannersd@sciex.com, (44) 191-374-2526, Fax (44) 191-374-2510.

SEPTEMBER 12-14, 2000

3rd UNITED KINGDOM MEETING ON COAL RESEARCH AND ITS APPLICATIONS
Birmingham, UK.

Information: H.J. Graham, Power Technology Centre, Radcliffe-on-Soar, Nottingham NG11 0EE, UK, 44(0)115-936-2460, Fax 44(0)115-936-2205, e-mail: helen.graham@powertech.co.uk

SEPTEMBER 13-16, 2000

2nd INTERNATIONAL CONFERENCE ON INORGANIC MATERIALS
Santa Barbara CA.

Information: Sarah Wilkinson, Conference Secretariat, Elsevier Science Ltd., The Boulevard, Langford Lane, Kidlington, Oxford, UK OX5 1GB, 44(0) 1865 843691, Fax 44(0) 1865 843658, e-mail: sm.wilkinson@elsevier.co.uk, http://www.elsevier.com/locate/im2000

SEPTEMBER 18-20, 2000

13th INTERNATIONAL SYMPOSIUM ON GAS FLOW AND CHEMICAL LASERS AND HIGH POWER LASER CONFERENCE
Florence, Italy.

Information: C. Pescucci, Fax 39(0) 55-233-7755, e-mail: gcl-hpl@ino.it, www.ino.it/GCL-HPL or www.es.titech.ac.jp/~kkasuya/gcl-web/index.html

SEPTEMBER 19-21, 2000

THE HYDROGEN ENERGY FORUM 2000
Munich, Germany.

Information: The Future Energies Forum, "Forum fur Zukunftsenergien", Godesberger Allee 90, D-53175 Bonn, Germany, Fax 49(0) 228-959 56-50, e-mail: energie.forum@t-online.de

SEPTEMBER 22-30, 2000

27th ANNUAL CONFERENCE OF THE FEDERATION OF ANALYTICAL CHEMISTRY AND SPECTROSCOPY SOCIETIES
Nashville TN.

Information: Division of Analytical Chemistry, FACSS, (505) 820-1648, Fax (505) 989-1073, Web Site: http://FACSS.org/info.html

SEPTEMBER 23-26, 2000

ASME FALL TECHNICAL CONFERENCE OF THE INTERNAL COMBUSTION ENGINE DIVISION
Peoria IL.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7054, Fax (212) 705-7143, http://www.asme.org

SEPTEMBER 24-26, 2000

1st ROMANIAN INTERNATIONAL CONFERENCE ON ANALYTICAL CHEMISTRY
Brasov, Romania.

Information: G.L. Radu, University of Bucharest, Faculty of Chemistry, 4-12, Elisabeta Blvd., Bucharest, Romania 703461, 40(1) 220 77 80/220 79 09, Fax 40(1) 220 76 95, e-mail: lucian@ibd.dbio.ro

SEPTEMBER 29-30, 2000

FOUR CORNERS SECTION FALL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Fort Collins CO.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 2-5, 2000

ICALEO 2000, INTERNATIONAL CONFERENCE ON APPLIED LASER APPLICATIONS AND ELECTROOPTICS
Dearborn MI.

Information: E. Cohen, Laser Institute of America, (800) 345-2737 or (407) 380-1553, Fax (407) 380-5588, http://www.laserinstitute.org

♦ OCTOBER 2-6, 2000

5th INTERNATIONAL AEROSOL SYMPOSIUM
Budapest, Hungary.

Information: N.N. Belov, Hungary, 1046 Budapest, Deak F. u., 26/a Belov N., Tel/Fax (36) 1-3791251, e-mail: belov@inext.hu, http://www.ias.inext.hu/uk-ias5-spo.htm.

OCTOBER 8-11, 2000

GASIFICATION TECHNOLOGIES CONFERENCE
San Francisco CA.

Information: M. Samoulides, (650) 855-2127, or Electric Power Research Institute, 1412 Hillview Avenue, Palo Alto, CA 94304, (650) 855-2599, http://www.epri.com

OCTOBER 13-14, 2000

OHIO SECTION FALL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Toledo, OH.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 16-19, 2000

INTERNATIONAL FUEL AND LUBRICANTS FALL MEETING AND EXPOSITION OF THE SOCIETY OF AUTOMOTIVE ENGINEERS
Baltimore MD.

Information: Society of Automotive Engineers, Inc., 400 Commonwealth Drive, Warrendale, PA 15096, (724) 776-4841, Fax (724) 776-5760, e-mail: meetings@sae.org, Web Site: http://www.sae.org

♦ OCTOBER 17-20, 2000

BEIJING INTERNATIONAL CONFERENCE ON APPLIED COMPUTATIONAL FLUID DYNAMICS
Beijing, China.

Information: Z. Tianyuan, Institute of Applied Physics and Computational Mathematics, (86) 10-62374357, Fax (86) 10-62010108, e-mail: zty@mail.iapcm.ac.cn, http://www.ciccst.org.cn/acfd

OCTOBER 19-20, 2000

SAMPLING, ON-SITE ANALYSIS AND SAMPLE PREPARATION CONFERENCE
Pittsburgh PA.

Information: B. Sherman, PACS, 409 Meade Dr., Coraopolis, PA 15108, (724) 457-6576 or (800) 367-2587, Fax (724) 457-1214, e-mail: hnpacs@aol.com, http://members.aol.com/hnpacs/pacs.htm

♦ OCTOBER 20-28, 2000

ANNUAL MEETING OF THE OPTICAL SOCIETY OF AMERICA AND THE INTERDISCIPLINARY LASER SCIENCE CONFERENCE
Providence RI.

Information: Optical Society of America, Meetings Department, 2010 Massachusetts Ave NW, Washington, DC 20036, (202) 223-0920, e-mail: confserv@osa.org, http://www.osa.org/mtg_conf
Deadline: Abstracts Due by May 16, 2000

OCTOBER 22-27, 2000

198th NATIONAL MEETING OF THE ELECTROCHEMICAL SOCIETY
Phoenix AZ.

Information: The Electrochemical Society, Inc., Meetings Department, 10 South Main Street, Pennington, NJ 08534, (609) 737-1902, Fax (609) 737-2743, e-mail: ecs@electrochem.org, http://www.electrochem.org/meetings/198/meet.html

OCTOBER 24-27, 2000

53rd ANNUAL GASEOUS ELECTRONICS CONFERENCE OF THE AMERICAN PHYSICAL SOCIETY
Houston TX.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 25-28, 2000

35th MIDWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
St Louis MO.

Information: C.D. Spilling, Department of Chemistry, University of Missouri, St. Louis, 80001 Natural Bridge Road, St. Louis, MO 63121 (314) 516-5313, Fax (314) 553-5342, e-mail: cspill@umsl.edu

OCTOBER 25-28, 2000

36th WESTERN REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
San Francisco CA.

Information: N.D. Byington, Customs Service Laboratory, 630 Sansome Street, Room 1429, San Francisco, CA 94111, (415) 705-4405 ext. 216, Fax (415) 705-4236, e-mail: byington@crl.com; or S. Rodriguez, Chemistry Department, University of the Pacific, Stockton, CA 95211, (209) 946-2598, Fax (209) 946-2607, e-mail: srodriguez@uop.edu

OCTOBER 28-29, 2000

JOINT FALL MEETING OF THE TEXAS SECTIONS OF THE APS, APPT AND ZONE 13 OF THE SPS
Houston TX.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

OCTOBER 29-NOVEMBER 3, 2000

EASTERN ANALYTICAL SYMPOSIUM OF THE AMERICAN CHEMICAL SOCIETY
Atlantic City NJ.

Information: S. Gold, Eastern Analytical Symposium, P.O. Box 633, Montchanin, DE 19710 (302) 738-6218, Fax (302) 738-5275, http://www.eas.org

NOVEMBER 1-2, 2000

COMPUTATIONAL AND EXPERIMENTAL METHODS IN RECIPROCATING ENGINES
London UK.

Information: U. Otuonye, Conference and Events Department C587, Institution of Mechanical Engineers, 1 Birdcage Walk, London SW 1H 9JJ, UK, (0) 207-304-6864, Fax (0) 207-222-9881, e-mail: u_otuonye@imeche.org.uk

NOVEMBER 2-4, 2000

SOUTHEAST SECTION MEETING OF THE AMERICAN PHYSICAL SOCIETY
Starkville MS.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

NOVEMBER 3-8, 2000

PHOTONICS EAST
Boston MA.

Information: Meetings Department, SPIE, P.O. Box 10, Bellingham, WA 98227, (360) 676-3290, Fax (360) 647-1445, e-mail: spie@spie.org, http://www.spie.org

NOVEMBER 5-10, 2000

ASME INTERNATIONAL MECHANICAL ENGINEERING CONFERENCE AND EXHIBITION
Orlando FL.

Symposia will Include:

- Symposium on Multiphase Flow in Biomedical Applications and Processes
- Dispersed Flows in Combustion, Incineration, and Propulsion Systems
- Application of Microfabrication to Fluid Mechanics

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 705-7037, Fax (212) 705-7143, http://www.asme.org

NOVEMBER 5-10, 2000

INTERNATIONAL SYMPOSIUM ON MULTIPHASE FLOW AND TRANSPORT PHENOMENA
Antalya, Turkey.

Topics will Include:

- Modeling of Multiphase Systems
- Transport Phenomena in Multiphase Systems
- Separation Phenomena, Processes and Equipment
- Measurement and Instrumentation
- Characteristic and Effective Properties of Multiphase Systems
- Bio-Aerosols and Bio-Systems
- Surface and Interfacial Phenomena
- Pollution Control Technology
- Clean Room Technology
- Multiphase Systems Applications
- Scaling Laws for Two-Phase Flow Phenomena
- Scaling Laws for Multiphase Flow

Information: D.M. Maron, Center for Technological Education Holon, POB 305, Holon 58102, Israel, (972) 3-502 6501, Fax (972) 3-502 6510, e-mail: barad_r@barley.cteh.ac.il, http://ichmt.me.metu.edu.tr/upcoming-meetings/MFTP-00/announce.html

NOVEMBER 5-10, 2000

UNITED ENGINEERING FOUNDATION CONFERENCE ON LEAN COMBUSTION TECHNOLOGY AND CONTROL
Santa Fe NM.

Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441, e-mail: engfnd@aol.com http://www.engfnd.org/engfnd/conf.html, or from D. Dunn-Rankin, University of California at Irvine, CA, or R.K. Cheng, Lawrence Berkeley National Laboratory.

NOVEMBER 12-17, 2000

ANNUAL MEETING OF THE AMERICAN INSTITUTE OF CHEMICAL ENGINEERS
Los Angeles, CA.

Information: Meetings Department, American Institute of Chemical Engineers, United Engineering Center, 3 Park Avenue, New York, NY 10016, (212) 591-7325, Fax (212) 591-8894, e-mail: meetmail@aiche.org, http://www.aiche.org

NOVEMBER 13-18, 2000

EASTERN ANALYTICAL SYMPOSIUM OF THE AMERICAN CHEMICAL SOCIETY
Somerset NJ.

Information: S. Gold, Eastern Analytical Symposium, P.O. Box 633, Montchanin, DE 19710, (302) 738-6218, Fax (302) 738-5275, Web Site: http://www.eas.org

NOVEMBER 19-21, 2000

DIVISION OF FLUID DYNAMICS MEETING OF THE AMERICAN PHYSICAL SOCIETY
Washington DC.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ NOVEMBER 19-23, 2000

4th EUROMECH FLUID MECHANICS CONFERENCE
Eindhoven, The Netherlands.

Information: M.C.J. Tielemans, Fluid Dynamics Laboratory, Department of Physics, Eindhoven University of Technology, P.O. Box 513, 5600 MB Eindhoven, The Netherlands, e-mail: info@efmc2000.tue.nl, http://www.EFMC2000.TUE.NL

NOVEMBER 27-DECEMBER 1, 2000

FALL MEETING OF THE MATERIALS RESEARCH SOCIETY
Boston MA.

Information: Materials Research Society, Meetings Department, 506 Keystone Drive, Warrendale, PA 15086, (724) 779-3003, Fax (724) 779-8313, http://www.mrs.org

DECEMBER 3-9, 2000

6th RIO SYMPOSIUM ON ATOMIC SPECTROMETRY
Concepcion and Pucon, Chile.

Information: C.G. Bruhn, Departamento de Analisis Instrumental, Facultad de Farmacia, Universidad de Concepcion, P.O. Box 237, Concepcion, Chile, (56) 41-204252, Fax (56) 41-231903, e-mail: cbruhn@udec.cl, http://www.udec.cl/6riosymp/

DECEMBER 6-8, 2000

JOINT 52nd SOUTHEAST/56th SOUTHWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
New Orleans LA.

Information: A. Pepperman, SRRC, USDA-ARS, 1100 Robert E. Lee Boulevard, New Orleans, LA 70179, (208) 286-4510, Fax (208) 286-4367, e-mail: abpep@nola.srrc.usda.gov

DECEMBER 14-19, 2000

INTERNATIONAL CHEMICAL CONGRESS OF PACIFIC BASIN SOCIETIES
Honolulu HI.

Information: Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

MARCH 4-8, 2001

THE PITTSBURGH CONFERENCE, PITTCON 2001
New Orleans LA.

Information: The Pittsburgh Conference, 300 Penn Center Boulevard, Suite 332, Pittsburgh, PA 15235, (412) 825-3220, Fax (412) 825-3224, e-mail: pittconinfo@pittcon.org, http://www.pittcon.org/

MARCH 12-16, 2001

ANNUAL MARCH MEETING OF THE AMERICAN PHYSICAL SOCIETY
Seattle WA.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

MARCH 25-30, 2001

199th NATIONAL MEETING OF THE ELECTROCHEMICAL SOCIETY
Washington DC.

Information: The Electrochemical Society, Inc., Meetings Department, 10 South Main Street, Pennington, NJ 08534, (609) 737-1902, Fax (609) 737-2743, e-mail: ecs@electrochem.org, http://www.electrochem.org/meetings/199/meet.html

♦ APRIL 1-5, 2001

221st NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
San Diego CA.

Division of Fuel Chemistry:

- CO_2 Capture and/or Utilization Reaction Mechanisms in Fuel Processing
  P.F Britt, Chemistry Division, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831, (423) 574-5029, Fax (423) 576-5235, e-mail: brittpf@ornl.gov
- Coal Bed Methane

P.C. Thakur, Consol Inc., R&D, 1027 Little Indian Creek Road, Morgantown, WV 26501, (304) 983-3207, Fax (304) 983-3209, e-mail: promodthakur@consolcoal.com

- Nitrogen Chemistry in Coal Utilization
  M.A. Wojtowicz, Advanced Fuel Research Inc., 87 Church Street, East Hartford, CT 06108, (860) 528-9806 ext 142, Fax (860) 528-0648, e-mail: marek@afrinc.com
- Hydrogen Energy
  R. Khan, Texaco Inc., P.O. Box 509, Beacon, NY 12508, (914) 838-7639, Fax (914) 838-7102
- Argonne National Lab Premium Coal Sample Database
  K. Vorres, 27 Windward Circle, Willowbrook, IL 60514, (630) 325-0931 [between Nov. 11 and April 15: 3432 North Applewood, Tucson, AZ 85712-5478, (520) 322-5256], e-mail: ksvorres@flash.net
- Carbon Products for Environmental Applications
  A. Lizzio, Illinois State Geological Survey, 615 East Peabody Drive, Champaign, IL 61801, (217) 244-4985, Fax (217) 333-8566, e-mail: lizzio@geoserv.isgs.uiuc.edu
- Fuels of the Future: Heavy Oil & Hydrogen for Fuel Cells
  R. Khan, Texaco Upstream Technology, 3901 Briar Park, Houston, TX 77042, (713) 954-6238, Fax (713) 954-6113, e-mail: khanmr@texaco.com
- Environmental Challenges for Fossil Fuel Combustion
  M.M. Maroto-Valer, Pennsylvania State University, Energy Institute, 405 Academic Activities Building, University Park, PA 16802, (814) 863-8265, Fax (814) 863-8892, e-mail: mmm23@psu.edu

APRIL 16-20, 2001

SPRING MEETING OF THE MATERIALS RESEARCH SOCIETY
San Francisco CA.

Information: Materials Research Society, Meetings Department, 506 Keystone Drive, Warrendale, PA 15086, (724) 779-3003, Fax (724) 779-8313, http://www.mrs.org

APRIL 23-27, 2001

APRIL NATIONAL MEETING OF THE AMERICAN PHYSICAL SOCIETY
Washington DC.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

♦ APRIL 29-MAY 2, 2001

INTERNAL COMBUSTION ENGINE DIVISION SPRING TECHNICAL CONFERENCE OF THE AMERICAN SOCIETY OF MECHANICAL ENGINEERS
Philadelphia PA.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7054, Fax (212) 705-7143, http://www.asme.org

MAY 6-11, 2001

CLEO/QELS 2001
Baltimore MD.

Information: Optical Society of America, Meetings Department, 2010 Massachusetts Ave NW, Washington, DC 20036, (202) 223-0920, e-mail: confserv@osa.org, http://www.osa.org/mtg_conf

MAY 20-25, 2001

FLUIDIZATION X
Beijing, China.

Information: United Engineering Foundation, Meetings Department, Three Park Avenue, 27th Floor, New York, NY 10016, (212) 591-7836, Fax (212) 591-7441, http://www.engfnd.org/engfnd/conf.html

MAY 20-25, 2001

2nd INTERNATIONAL SYMPOSIUM ON ADVANCES IN COMPUTATIONAL HEAT TRANSFER
Cairns, Australia.

Information: F. Arinc, Secretary-General, ICHMT, Mechanical Engineering Department, Middle East Technical University, 06531 Ankara, Turkey, (90) 312-210-1429, Fax (90) 312-210-1331, arinc@metu.edu.tr, http://ichmt.me.metu.edu.tr

♦ MAY 27-JUNE 1, 2001

4th INTERNATIONAL CONFERENCE ON MULTIPHASE FLOW
New Orleans LA.

Information: E.E. Michaelides, School of Engineering, Tulane University, New Orleans, LA 70118, e-mail: icmf@mailhost.tcs.tulane.edu, http://mail.eng.lsu.edu/icmf.2001/
Deadline: Abstracts Due by July 1, 2000

MAY 30-JUNE 1, 2001

35th MIDDLE ATLANTIC REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Baltimore MD.

Information: L.J. Boucher, Towson University, Department of Chemistry, 8000 York Road, Towson, MD 21252-0001, (410) 830-3057, Fax (410) 830-4265, e-mail: lboucher@towson.edu

♦ JUNE 4-7, 2001

ASME TURBO EXPOSITION: LAND, SEA AND AIR
New Orleans, LA.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (404) 847-0072, Fax (212) 705-7143, http://www.asme.org

♦ JUNE 10-15, 2001

3rd INTERNATIONAL SYMPOSIUM ON RADIATIVE TRANSFER
Antalya, Turkey.

Information: F. Arinc, Secretary-General, ICHMT, Mechanical Engineering Department, Middle East Technical University, 06531 Anakara, Turkey, (90) 312-210-5214, Fax (90) 312-210-1331, http://ichmt.me.metu.edu.tr
Deadline: 4 Copies of Manuscript Due by December 15, 2000.

JUNE 11-13, 2001

JOINT CENTRAL/GREAT LAKES REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Grand Rapids MI.

Information: R.J. McCabe, Parke-Davis Pharmaceuticals, 188 Howard Ave., Holland, MI 49424, (616) 392-2375 ext. 2386, Fax (616) 392-8916, e-mail: Richard.McCabe@wl.com

JUNE 13-15, 2001

JOINT 33rd CENTRAL/33rd GREAT LAKES REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Grand Rapids MI.

Information: R.J. McCabe, Parke-Davis, 188 Howard Avenue, Holland, MI 49423, (616) 392-2375 ext 2386, Fax (616) 392-8916, e-mail: Richard.McCabe@wl.com

JUNE 13-16, 2001

56th NORTHWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Seattle WA.

Information: S. Jackels, Department of Chemistry, Seattle University, 900 Broadway, Seattle, WA 98122, (206) 296-5946, Fax (206) 296-5786, e-mail: sjackels@seattleu.edu

JUNE 24-27, 2001

30th NORTHEAST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Durham NH.

Information: H. Mayne, Chemistry Department, University of New Hampshire, (603) 862-1550, e-mail: howard.mayne@unh.edu

JUNE 24-28, 2001

ANNUAL MEETING OF THE AIR AND WASTE MANAGEMENT ASSOCIATION
Orlando FL.

Information: Air and Waste Management Association, Member Services, One Gateway Center, Third Floor, Pittsburgh, PA 15222, (800) 270-3444 or (412) 232-3444, Fax (412) 232-3450, http://www.awma.org

JULY 1-6, 2001

GORDON RESEARCH CONFERENCE ON LASER DIAGNOSTICS IN COMBUSTION
Mount Holyoke College, South Hadley MA.

Information: J.B. Jeffries, Molecular Physics Laboratory, SRI International, 333 Ravenswood Ave., Menlo Park, CA 94025, (650) 859-6341, Fax (650) 859-6196, e-mail: jay.jeffries@sri.com

JULY 9-11, 2001

COMBUSTION CHEMISTRY: ELEMENTARY REACTIONS TO MACROSCOPIC PROCESSES: FARADAY DISCUSSION NUMBER 119
Leeds, UK.

Joint Meeting with the British Section of the Combustion Institute.
Information: M. Pilling, School of Chemistry, University of Leeds, Leeds UK, e-mail: m.j.pilling@chem.leeds.ac.uk, http://www.chem.leeds.ac.uk

♦ JULY 29-AUGUST 2, 2001

36th INTERSOCIETY ENERGY CONVERSION ENGINEERING CONFERENCE
Savannah GA.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7057, Fax (212) 705-7143, http://www.asme.org

♦ AUGUST 19-24, 2001

1st INTERNATIONAL CONFERENCE ON ADVANCED VIBRATIONAL SPECTROSCOPY
Turku, Finland.

Information: M. Hotokka, Department of Physical Chemistry, Abo Akademi University, FIN-20500 Turku, Finland, 358-2-215-4295, Fax 358-2-215-4706, e-mail: icavs@abo.fi, http://www.abo.fi/icavs

AUGUST 20-24, 2001

13th INTERNATIONAL CONFERENCE ON FOURIER TRANSFORM SPECTROSCOPY
Turku, Finland.

Information: M. Hotokka, Department of Physical Chemistry, Abo Akademi University, FIN-20500 Turku, Finland, (358) 2-265-4295, Fax (358) 2-265-4706, e-mail: icofts@abo.fi, http://www.abo.fi/icofts

♦ AUGUST 26-30, 2001

222nd NATIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Chicago IL.

Division of Fuel Science:

- Cofiring or Coprocessing Coal & Biomass
  J.T. Cobb, Jr., University of Pittsburgh, Chemical Engineering Department, 1137 Benedum Hall, Pittsburgh, PA 15261, (412) 624-7443, Fax (412) 624-9639, e-mail: cobb@engrng.pitt.edu
- Computer Modeling in Fuel Chemistry
  J. Mathews, Pennsylvania State University, Energy & Geo-Environmental Engineering Department, 151 Hosler Building, University Park, PA 16802, (814) 863-6213, Fax (814) 865-3248, e-mail: jpm10@psu.edu; M.T. Klein, Rutgers, State University of New Jersey, School of Engineering, Office of the Dean, B204, 98 Bret Road, Piscataway, NJ 08854-8058, (732) 445-4453, Fax (732) 445-7067, e-mail: mtklein@jove.rutgers.edu
- Fine Particulate (PM2.5) Formation & Emissons from Fuel Combustion
  C.M. White, Department of Energy, Federal Energy Technology Center, Mail Stop 94-212, P.O. Box 10940, Pittsburgh, PA 15236, (412) 386-5808, Fax (412) 386-4158, e-mail: cwhite@fetc.doe.gov
- Catalysis in Fuel Processing for Fuel Cell Application
  S.P. Katikaneni, Fuel Cell Energy, Advanced Technology Group, 3 Great Pasture Road, Danbury, CT 06813, (203) 825-6067, Fax (203) 825-6150, e-mail: skatikaneni@fce.com; A.M. Gaffney, DuPont Central R&D, Experimental Station, P.O. Box 80262, Wilmington, DE 19880, (302) 695-1800, Fax (302) 695-8347, e-mail: anne.m.gaffney@usa.dupont.com; C. Song, Pennsylvania State University, Energy & Geo-Environmental Engineering, 206 Hosler Building University Park, PA 16802, (814) 863-4466, Fax (814) 865-3248, e-mail: csong@psu.edu
- Value-Added Carbon Products from Fossil Fuels
  F. Rusinko, Pennsylvania State University, Energy Institute 407 Academic Activities Building, University Park, PA 16802, (814) 863-8085, Fax (814) 865-8892, e-mail: fjr4@psu.edu; J.W. Zondlo, College of Engineering & Mineral Resources, Department of Chemical Engineering, P.O. Box 6102, Morgantown, WV 26506; B. Tomer, Department of Energy, Federal Energy Technology Center, 3610 Collins Ferry Road, P.O. Box 88, Morgantown, WV 26507.
- Mercury Emissions from Coal
  K. Katrinak, Microbeam Technologies, 1521-24th Avenue S., Suite B-2, Grand Forks, ND 58201, (701) 772-4482, Fax (701) 772-4099, e-mail: katrinak@badlands.nodak.edu; K. Galbreath, University of North Dakota, Energy & Environmental Research Center, P.O. Box 9018, Grand Forks, ND 58202, (701) 777-5127, Fax (701) 777-5181, e-mail: kgalbreath@eerc.und.nodak.edu
- General Fuel Chemistry
  S.V. Pisupati, Pennsylvania State University, Energy & Geo-Environmental Engineering, 124 Hosler Building, University Park, PA 16802, (814) 865-0874, Fax (814) 865-3248, e-mail: sxp17@psu.edu

Information: Meetings Department, American Chemical Society, 1155 - 16th Street, NW, Washington, DC 20036, (202) 872-4396, Fax (202) 872-6128, e-mail: natlmtgs@acs.org

Deadline: Electronic Abstract Submissions (preferred) or 4 Hard Copies of 150-word Abstract (original on ACS Abstract Form) Due to Symposium Organizers by April 15, 2001. Preprints Due to Symposium Chairs by May 15, 2001.

SEPTEMBER 2-7, 2001

200th NATIONAL MEETING OF THE ELECTROCHEMICAL SOCIETY AND THE 52nd MEETING OF THE INTERNATIONAL SOCIETY OF ELECTROCHEMISTRY
San Francisco CA.

Information: The Electrochemical Society, Inc., Meetings Department, 10 South Main Street, Pennington, NJ 08534, (609) 737-1902, Fax (609) 737-2743, e-mail: ecs@electrochem.org, http://www.electrochem.org/meetings/198/meet.html

SEPTEMBER 23-27, 2001

52nd SOUTHEAST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Savannah GA.

Information: G. Novotnak, Kemira Pigments, 104 Carlton Road, Savannah, GA 31410, (912) 652-1290, Fax (912) 897-1163, e-mail: george.novotnak@kemira.com

SEPTEMBER 23-27, 2001

6th WORLD CONGRESS OF CHEMICAL ENGINEERING: A NEW CENTURY OF CHEMICAL ENGINEERING
Melbourne, Australia.

Information: Meetings Department, American Institute of Chemical Engineers, United Engineering Center, 3 Park Avenue, New York, NY 10016, (212) 591-7325 or (800) 242-4363, Fax (212) 591-8894, e-mail: meetmail@aiche.org, http://www.aiche.org

♦ SEPTEMBER 24-26, 2001

INTERNAL COMBUSTION ENGINE DIVISION FALL TECHNICAL MEETING OF THE AMERICAN SOCIETY OF MECHANICAL ENGINEERS
Argonne IL.

Information: Meetings Department, American Society for Mechanical Engineers, 345 E. 47th Street, New York, NY 10017, (212) 591-7054, Fax (212) 705-7143, http://www.asme.org

♦ SEPTEMBER 24-28, 2001

5th WORLD CONFERENCE ON EXPERIMENTAL HEAT TRANSFER, FLUID MECHANICS AND THERMODYNAMICS
Thessaloniki, Greece.

Information: G.P. Celata, Conference Chairman, ENEA Casaccia, Via Anguillarese 301, I-00060 S.M. Galeria, Rome, Italy, (39) 06-30483905, Fax (39) 06-30483026, e-mail: celata@casaccia.enea.it, http://www.ing.unipi.it/exhft5
Deadline: Abstract Due by July 28, 2000

OCTOBER 5-12, 2001

28th ANNUAL MEETING OF THE FEDERATION OF ANALYTICAL CHEMISTRY AND SPECTROSCOPY SOCIETIES
Detroit MI.

Information: C. Lilly, Federation of Analytical Chemistry and Spectroscopy Societies, 1201 Don Diego Ave., Santa Fe, NM 87505, (505) 820-1648, Fax (505) 989-1073, e-mail: jsjoberg@trail.com, http://facss.org/info.html

OCTOBER 10-13, 2001

36th MIDWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Lincoln NE.

Information: D. Berkowitz, Department of Chemistry, University of Nebraska, Lincoln, NE 68588-0304, (402) 472-2738, Fax (402) 472-9402, e-mail: dbb@unlinfo.edu

OCTOBER 14-19, 2001

INTERNATIONAL SYMPOSIUM ON VISUALIZATION AND IMAGING IN TRANSPORT
Antalya, Turkey.

Information: F. Arinc, Secretary-General, ICHMT, Mechanical Engineering Department, Middle East Technical University, 06531 Ankara, Turkey, (90) 312-210-1429, Fax (90) 312-210-1331, arinc@metu.edu.tr, http://ichmt.me.metu.edu.tr

OCTOBER 16-19, 2001

57th SOUTHWEST REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
San Antonio TX.

Information: S.T. Weintraub, Department of Biochemistry, University of Texas Health Science Center, 7703 Floyd Curl Drive, San Antonio, TX 78284, (210) 567-4043, Fax (210) 567-5524, e-mail: weintraub@uthscsa.edu

OCTOBER 23-26, 2001

36th WESTERN REGIONAL MEETING OF THE AMERICAN CHEMICAL SOCIETY
Ventura CA.

Information: R.W. Hurst, 9 Faculty Court, Thousand Oaks, CA 91360, (805) 492-7764, Fax (805) 241-7149, e-mail: Alarwh@aol.com

NOVEMBER 26-30, 2001

FALL MEETING OF THE MATERIALS RESEARCH SOCIETY
Boston MA.

Materials Research Society, Meetings Department, 506 Keystone Drive, Warrendale, PA 15086, (724) 779-3003, Fax (724) 779-8313, e-mail: info@mrs.org

♦ MARCH 18-22, 2002

MARCH MEETING OF THE AMERICAN PHYSICAL SOCIETY
Indianapolis IN.

Information: American Physical Society, Meetings Department, One Physics Ellipse, College Park, MD 20740, (301) 209-3280, Fax (301) 209-0867, http://www.aps.org

CURRENT BIBLIOGRAPHY RELEVANT TO
FUNDAMENTAL COMBUSTION
December 1999

Keith Schofield, ChemData Research, P.O. Box 40481
Santa Barbara, CA 93140, (805) 966-7768, Fax (805) 893-8797
e-mail: combust@mrl.ucsb.edu
http://www.ca.sandia.gov/CRF/Publications/CRB/CRB.html

1. FUELS/SYNFUELS - GENERAL

83378.	Wang, X., "The Consideration and Choice on Exploiting Energy Source," *Chinese Sci. Bull.* 44, 1717-1728 (1999).	Energy Sources Future Global Strategies
83379.	Sayigh, A., "Renewable Energy: The Way Forward," *Appl. Energy* 64, 15-30 (1999).	Renewable Energy Potential Global Energy Needs Review
83380.	Datschefski, G., "Future Trends in Fuels," in *Aeroengines and Propulsion*, 9 Papers, 92 pp., *I.Mech.E. Seminar Publications*, No. 12, 65-72 (1996).	Aircraft Fuels Future Trends Kerosine Role
83381.	Drayton, M.K., A.V. Saveliev, L.A. Kennedy, A.A. Fridman and Y.E.(David) Li, "Syngas Production Using Superadiabatic Combustion of Ultrarich Methane/Air Mixtures," *Symp. (Int.) Combust. Proc.* 27, 1361-1367 (1998).	Syngas Formation Ultrarich CH_4/Air Partial Oxidation Filtration Combustion Method CO,H_2 Yields
83382.	Chen, Y., S. Charpenay, A. Jensen, M.A. Wojtowicz and M.A. Serio, "Modeling of Biomass Pyrolysis Kinetics," *Symp. (Int.) Combust. Proc.* 27, 1327-1334 (1998).	Biomass Pyrolysis Products Kinetics Model Development
83383.	Choudhuri, A.R., and S.R. Gollahalli, "Laser Induced Fluorescence Measurements of Radical Concentrations in Hybrid Gas Fuel Flames," pp. 489-496 in *Proceedings of the 1997 International Joint Power Generation Conference. Volume 1. Environmental Control/Fuels and Combustion Technologies/Nuclear Engineering*, A. Sanyal, A. Gupta and J. Veilleux, eds., 77 Papers Presented in Denver CO, November 1997, ASME Publication EC-Vol. 5, 678 pp., The American Society of Mechanical Engineers, New York (1997).	Natural Gas/H_2 Fuel Mixture CH,CN,OH,LIF Measurements Hybrid Fuel Effects

83384. Li, X., J.-S. Chang and S.-E. Park, "Carbon as an Intermediate during the Carbon Dioxide Reforming of Methane over Zirconia-Supported High Nickel Loading Catalysts," *Chem. Lett. Jpn.* 1099-1100 (1999).

CH_4/CO_2
Catalytic
Reforming
Ni/ZrO_2
Effectiveness

83385. Malik, M.A., and X.Z. Jiang, "The CO_2 Reforming of Natural Gas in a Pulsed Corona Discharge Reactor," *Plasma Chem. Plasma Process.* 19, 505-512 (1999).

CH_4/CO_2
Fuel Reforming
Pulsed Discharge
CO/H_2 Formation

2. LIQUEFACTION/GASIFICATION

83386. Yoshikawa, K., T. Ootsuka, H. Katsushima, T. Hasegawa, R. Tanaka, T. Kiga and K. Makino, "High Temperature Air Coal Combustion Utilizing Multi-Staged Enthalpy Extraction Technology," pp. 279-285 in *Proceedings of the 1997 International Joint Power Generation Conference. Volume 1. Environmental Control/Fuels and Combustion Technologies/Nuclear Engineering*, A. Sanyal, A. Gupta and J. Veilleux, eds., 77 Papers Presented in Denver CO, November 1997, ASME Publication EC-Vol. 5, 678 pp., The American Society of Mechanical Engineers, New York (1997).

Coal Gasifier
High Temperature
Air
Pebble Bed
Ash Removal

83387. Shah, N., J. Rockwell and G.P. Huffman, "Conversion of Waste Plastic to Oil: Direct Liquefaction versus Pyrolysis and Hydroprocessing," *Energy Fuels* 13, 832-838 (1999).

Liquefaction
Waste Plastics
2 Approaches
Catalyst
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83388. Joo, H.K., J.N. Hool and C.W. Curtis, "Determination of Effective Conditions for Two-State Coprocessing of Coal with Waste Plastics and Petroleum Resid," *Energy Fuels* 13, 1128-1134 (1999).

Liquefaction
Gasification
Plastic Wastes/
Coal/Petroleum
Catalytic
Multistaged
Process

(83446) Gasification Pyrolysis, Kinetic Model

Polystyrene

83389. Dasappa, S., P.J. Paul, H.S. Mukunda and U. Shrinivasa," Wood Char Gasification: Experiments: and Analysis on Single Particles and Packed Beds," *Symp. (Int.) Combust. Proc.* 27, 1335-1342 (1998).

Gasification
Wood Char/H_2O
Modeling

83390. Androulakis, I.P., and S.C. Reyes, "Role of Distributed Oxygen Addition and Product Removal in the Oxidative Coupling of Methane," *AIChE J.* 45, 860-868 (1999).

Partial Oxidation
CH_4/O_2
C_2 Product Yield
Optimization
Staged O_2
Addition Method
Model

83391. Teng, Y., F. Ouyang, L. Dai, T. Karasuda, H. Sakurai, K. Tabata and E.

Partial Oxidation

	Suzuki, "High Yield Methanol Formation in a $CH_4/O_2/NO_2$ Gaseous Selective Oxidation at 1 atm," *Chem. Lett. Jpn.* 991-992 (1999).	CH_4/CH_3OH Conversions $CH_4/O_2/NO_2$ Products,Yields

3. BURNERS

(See also Section 21 for Burner Emissions and Incinerator Performance)

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Biomass Fuel
Fly Ash Deposition
Efficiencies
Sizes

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FBC
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Bed Ash
Agglomeration
Characteristics

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Circulating
Industrial Wastes
Numerical
Model

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Pulverized Coal
Combustion
Char Incomplete
Burnout
Mechanism

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Carbon Particle
Combustion
Transition Phase
Burnout
Radius Effects

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Coal,Anthracene
Pyrolysis
Benz(f)indene
Formation

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Coal/Biomass
Cofiring
NO_x Emissions
Ash,Corrosion

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Spray Flame

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Fuel Spray
PDA,PIV
LIF Imaging
Sizes,Velocities
Stratified
DI Engines

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Sizes,Velocities
In Cylinder
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Spray Flames
Enclosed
Ignition
Combustion
CFD Modeling

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Spray Combustion
Enclosed Chamber
Gravity Effects
Flame Length
Modeling

(83509) Instabilities, Active Control, Low CO, NO_x Emissions

Liquid Fueled
Combustor

(83730) NO Formation, Fuel Sulfur Effects, Kinetic Modeling

Gas Oil Spray
Flame

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Swirl Spray
Combustor
EGR Effects
NO Formation

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Spray Combustion
CCl_3CH_3/C_7H_{16}
$CCl_3CH_3/C_{16}H_{34}$
Density Effects
Destruction
Efficiencies

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(83943)	Temperatures, OH, NO Absorption, Pulsed Xe Lamp, CCD Detector	Propellant Combustion
(84047)	Unimolecular Dissociation, Channels, HONO, NO_2 Products, Energies, Dynamics	$(CH_3)_2NNO_2$
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(84050)	Unimolecular Dissociation, Collision Activation Limited Step, Rate Constants, Model	RDX
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(84189)	ΔH_f , Calculations	$N(NO)_3$,$NH(NO)_2$ NH_2NO,NH_2NO_2
(83976)	Pyrolysis Mechanism	$NH_4N(NO_2)_2$
(83469)	Spontaneous Ignition, Heated Fuel, Gravity Effects, Model	Solid Fuel
(83566) (83567) (83568)	Inhibition Techniques, Conference Proceedings	Polymer Combustion

(83467) Auto-ignition Temperatures, $\Delta H_{combustion}$ — Epoxy,Phenolic Imide,Vinyl Ester Composites

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MHD
Coal Fired
Laser Induced
Breakdown Spectra
Particles
Atomic Analysis

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Temperatures
Thermocouples
Turbulent Jet
Measurements

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Temperatures
Pyrometer
Multiwavelength
1500-6000 K
CH_3NO_2 Detonations

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Temperatures
Laser Interferometric
2-D Holography
CH_4/Air

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Temperatures
Speckle Tomography
Multijet
Turbulent Flame

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Temperatures
IR Emission
Tomography
Heated Gas Flows
Algorithm

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Temperatures
Rotational
CH(A-X)
Emission Spectra
CH_4,C_2H_4,C_2H_2/O_2
Flames

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Temperatures
Phosphor Materials
Surfaces
≤700 °C

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Temperatures
Phosphor
Phosphorescence
Heated Surfaces
300-1300 K
Uncertainties

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Temperatures
Fluorescence
2-Methods
Intensity Ratio
Lifetime
Sensitivities

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Temperatures
Dye,LIF
2-D LDA
Turbulent Jet
Measurements

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Temperatures
Fluorescence
Slice Imaging
$C_{10}H_{22}$ Droplet in
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Composites
Temperatures
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Electrostatic
Ignition

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Ignition/
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Ignition

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Inhomogeneous
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Ignition

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Chain Branching
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Theory

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Conditional Moment Closure

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Alignments

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PLIF,OH

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Turbulent Jet
Steady Crossflow
PLIF
Fractal
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2-Point
Rayleigh
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Mechanism

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Numerical Model

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Modeling
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Inadequacies

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CH_4 Jet
Nonpremixed
Lift-off Heights
Blowoff Velocities
High Strain
Modeling

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CH_4/Air
H_2/Ar/Air
ps LIF,OH
Quantitative
Measurements

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Cold H_2 Jet
Counterflowing
Heated Air Jet
Measurements

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New Models

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Cell Size
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Detonations
Jet Initiation
Mechanisms

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(83952) Monitor, Laser Photofragmentation Method | Nitro-Explosives

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(83907)	Atmospheric Airborne Monitors, 40 Years Experience, Review	Mass Spectrometers
(83908)	Low Pressures, Coupled Gas Chromatography, Molecular Beam/Mass Spectrometer Technique, Complementary Aspects	Flame Monitor
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(83909) CH_4 Discharge, Quadrupole Mass Analyzer, C_1, C_2, C_3 and H_2 Fragment Ions Monitor — CH_3; Ion Fragments

(83910) Radical Mass Analysis, Telluride Conversion Method — CH_3,CF_3,CF_2H; CH_2F,C_2F_5,F

(84039) Singlet/Triplet P.E. Surfaces, Unimolecular Dissociation, Rate Constants, RRKM Calculations — CH_3S^+

(84040) Unimolecular Dissociation, Channels, Rate Constants, RRKM Calculations — CH_3SH^+

(83778)	Radiofrequency Discharge, Ions, Diamond Formation, Mass Spectral Analysis	CH_4/O_2
(84062)	Reaction Dynamics, P.E. Surfaces, Rates, Calculations	$C_2H_2^+ + CH_4$
(84042)	Unimolecular Dissociation, Product Energy Release	$C_2H_3Br^+$
(84048)	Isomerization, P.E. Surfaces, Low-lying States, Linear/Bent Structures, Calculations	C_3^-, C_3
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(83799)	Rate Constants, M = Numerous Inorganic or Organic Molecules, Channels, Review	$C_{60}^+ + M + He$
(84074)	Reaction Dynamics, P.E. Surfaces, Energies, Transition States	$Co^+, Co^{*+} + H_2O$ $Cu^+, Cu^{*+} + H_2O$ $Ni^+, Ni^{*+} + H_2O$
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(84083)	Reaction Dynamics, Calculations, HCN/HNC Product Mechanisms	$N^+ + CH_3$ $N + CH_3^+$ $CH_2N^+ + e^-$
(84020)	2-Photon Above Threshold Dissociation, Calculations	$Na_2^+ + h\nu_1 + h\nu_2$ $Li_2^+ + h\nu_1 + h\nu_2$
(83896)	Transition Probabilities, Calculations	Ne^+(3d-3p)
(83801)	Rate Constants, Product Ions	$Ni_n^+ + NO$ $Ni_nO_m^+ + NO$
(84036)	Product OH^-(v), OD^-(v) Energies, Collision Energy Effects	$O^- + H_2, D_2$

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(83802)	Photodissociation Products, Branching Ratios, Mass Analysis, n=1-4, m=1-6	$Sr^+(H_2O)_n + h\nu$ $Sr^+(D_2O)_m + h\nu$
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(83613)	Diesel Engine Exhaust, NO Control Method	CH_3NH_2 Additive
(83757)	Additive Effects, Soot Formation, Diffusion Flames, Volume Fractions, Smoke Heights, Temperature Dominant Role	CS_2,H_2,O_2
(83970)	$CH_4/O_2/Ar$ Flames, Species Profiles, Major Channels, Kinetic Model	C_2HCl_3 Inhibition

(83961)	C_2H_6/H_2/Air Flames, Species Profiles, Mechanisms	C_3HF_7 Inhibition
(83971)	CH_4/O_2 Flames, Species Profiles, Measurements, Kinetic Modeling Comparisons	C_3HF_7 Inhibition
(83770)	Soot Formation, C_2H_4/Air, Counterflow Flames, PAH Profiles	C_3H_8, O_2 Additive Effects
(83413)	As, Hg, Se Speciation, Coal Combustion, Equilibrium Calculations, AsSe, HgSe Roles	Cl Effects
(83604)	Diesel Engines, Soot Control, Copper Catalytic Filter Comparisons	Cu Fuel Additives
(83772)	Soot Formation, C_2H_4 Pyrolysis, Shock Tube	$Fe(CO)_5$ Effects
(83483)	C_3H_8 Combustion, High Temperature Preheated Air, Ionic Species Mass Analysis	Li Additive

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Fuel Blends
Performance
UHC,NO Emissions

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Auto Development
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Measurements

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Fuel Additives
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UHC,Soot
NO_x Emission
Effects

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Performance
CO,HC,NO_x ,Soot
Emissions

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$(CH_3)_2O$ Fuel
Simulated Exhaust
NO_x Catalysts
Performance

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Pre-,Main Injection
Variation Effects
NO_x ,Soot
Emissions

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Speed Effects
NO_x ,Soot
Emissions

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Fuel Injection
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Effects
NO_x ,Soot Control

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CH_3NH_2
Exhaust Additive
NO Control
Method

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Northern Latitudes
CO,HC,HCl
O_3 ,N Species,Ice
Aircraft Monitoring
Heterogeneous
Ice/Cl Formation
O_3 Destruction

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CO_2
Sinks
1000 Year History

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$(CHF_2)_2O$
$(CF_3CH_2)_2O$

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Intercomparisons
29 Groups

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HCOOH
Sources,Sinks
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Troposphere
CH_3COOH,HCOOH
$(CH_3)_2CO$
Measurements

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Stratospheric
Tropospheric
$(CH_3)_2CO$
Measurements

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$ClNO_2$,HCl
Heterogeneous
Sea Salt Source
Inventory

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Measurements
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HO_2,OH
3-D Modeling
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HO_2,OH
Twilight
New Observed Source
HNO_3,HNO_4
Suggestion

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HO_2,RO_2
Peroxy Monitor
Mixing Ratios
RO_2/H_2SO_4
Conversion Method

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H_2
Mixing Ratio
Sources,Sinks
Budget

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Ice Particle
Formation
Soot/H_2SO_4
Activation Nuclei

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Aerosols
Aircraft Emission
Source

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Sources
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IO_2
Stability
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Role

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Tropospheric
NO_x
Global Model
Sources,Sinks
Adequacies

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Aircraft Emissions
NO_x

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Stratospheric
NO_x,NO_y
Measurements/
Modeling
Comparisons

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Tropospheric
NO_x,NO_y
$(CH_3)_2CO$,Peroxy
Model Source
Effects

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NO_x /OH,HO_2

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NO_x ,O_3
Modeling
O,OH + NO_2
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New Rate Constant
Effects

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Reliabilities

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N_2O
O-Atom Isotopic
Ratios
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Formation
Dominance

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O_3
Budget
Heterogeneous
Aerosol Chemistry
$BrONO_2$,$ClONO_2$
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Stratospheric
O_3
Br Destructive
Effectiveness

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O_3
NO_x /VOC
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Pb
Historical
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Climatic Change
CH_4 ,CO,NO_x ,N_2O
Halocarbons
Greenhouse
Warming
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NO Control
Asbestos
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Turbulence
Effects

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Efficiencies

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Temperature
Effects

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Gas Turbine
Cycle Loop
O_2/Recycled CO_2

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FE-36,FM-200
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Turbulent
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O_2 Enriched Air
Performance

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Adequacies

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Pulverized Coal
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Mechanisms

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Gas Turbine
Natural Gas Fuel
Lean Burn
Parameter Effects

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Modeling

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Turbulent
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Effects
Scaling

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NO Formation
$CH_4/O_2/N_2$
CH,NO,LIF
Measurements
Modeling
Reburn Chemistry

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CH_4/Air
Counterflow Flame
O_2 Enriched
Effects

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CH_4/Air
Counterflow
Flames
LIF,NO
Kinetic Modeling

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CO,NO_x Formation
Swirling CH_4
Jet Flame
Fuel/Air
Mixing Effects
2-D LIF,OH
LDV

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Lean CH_4/Air
Stirred Reactor
Pressure Effects
Measurements

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CH_4, C_2H_6/Air
LIF Measurements
Kinetic Modeling
Inadequacies

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NO Formation

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CO,NO
Emissions
C_3H_8, $(CH_3)_2O$
n-C_4H_{10} Flames
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Turbulent
C_3H_8 Jet Flame
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NO Emissions

(83492) Flame/Surface Interactions, H_2/Air, Thermal Quenching, Model

H_2, NO_x Emissions

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Overfire Air
Coal Fuels
Performance

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Regenerative
Burner
Modeling

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Highly Preheated
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Efficiencies

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NO_x Control

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NO_x Control
Thermal $DeNO_x$
NH_3 Method
Stirred Reactor
Partial Pressure
Effects

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NO Control
Thermal $DeNO_x$
NH_3 Method
Na_2CO_3 Additive
Enhancement
Effects
Measurements

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NO_x Control
Reburn Method
HC/NH_3 Injection
Reduced Scheme
Predictive
Kinetic Model

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NO Control
Reburn Method
Natural Gas
Injection
Mixing Effects

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CO,Organics
NO_x Control
Natural Gas
Reburn Method
Incineration
Solid Wastes

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NO_x Control
Reburn Method
Micronized Coal Injection
Performance

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Reburn Methods
Pilot Scale Tests
Efficiencies
Na Additive Effects

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NO_x Control
Catalytic Methods
Overview

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Gas Turbine
Catalytic Combustion
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NO_x Control
Corona Discharge Method
NO_2 Removal
H_2O Effects

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NO Control

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NO_x Control
Flue Gases
Photo-triggered Discharge Method

22. SOOT, DIAMOND, PARTICLE FORMATION/CONTROL

(See also Section 19 for Soot Formation in Engines)

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Soot Formation
PAH Growth
C_2H_2, C_6H_6
Pyrolysis
Measurements
Modeling

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Soot Formation
C_2H_4/O_2
Precursor Channels
Kinetic Modeling
Species Profiles

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Soot Formation
Growth Model
Volume Fractions
Probe,Optical
Measurements
C_2H_4 Diffusion
Coflow Flame

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Soot Formation
C_2H_4/Air
Stirred Reactor
Kinetic Model
Dominant
Features

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C_2H_4/Air
Scattering/
Extinction
Aggregates
Measurements

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Soot,PAH
Formation
Rich C_2H_4/Air
Jet Stirred Reactor
CO_2, N_2 Addition
Effects

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Soot Formation
C_2H_4/Air
Counterflow Flames
C_3H_8, O_2 Additive
Effects
PAH Profiles

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Soot Formation
C_2H_4/Air
Volume Fractions
LII,Extinction
T,N_2 CARS
Modeling
Deficiencies

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Soot Formation
C_2H_4
Pyrolysis
$Fe(CO)_5$ Effects
Shock Tube

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Soot Aerosol

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Diamond Like
Materials
Growth
Nucleation
Monograph

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Graphitic Carbon
$CH_4/H_2/O_2$
ECR Plasma

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CH_4/H_2
Microwave Discharge
Xe Enhancement
Effects
Mechanism

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Diamond Formation
CH_4/H_2/Ar
dc Discharge
H Impurities
Defects

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CH_4/H_2/(CO)
ICP Plasmas
C,CH,OH,H
Monitoring
C-Atom Role

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Diamond Formation
CH_4/O_2
RF Discharge
Ions Analysis

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C_2H_2/O_2
Gas/Surface
Kinetic Modeling
Growth Rates
H-Atom Effects

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Aerosol Formation

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Particle Formation

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Al_2O_3 Particles
Flame Synthesis
Surface Areas
Measurements
Modeling

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Ice Particle Formation

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Si
Particle Formation
SiF_4,SiH_4/H_2
Glow Discharges

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Growth
SiH_4 Discharge
Measurements

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Si
Particle Formation
SiH_4 Discharge
Size,Density

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Si
Nanoparticles
Raman,LIF
Monitoring
Nucleation,Growth
IR MPD SiH_4

23. PARTICLE CHARACTERIZATION

(See also Section 5 for Spray Characterization)

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Plasma Discharge
Thermophoretic Force
Analysis

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Fly Ash
Carbon Content
Diffuse
Reflectivity
Method

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Fly Ash
PAH Content
FB Gasification
Wood Biomass
Textile Wastes
Feedstock
Dependence

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Fly Ash
Na_2SO_4,NaCl
Salt Content
Sizes
Measurements
Recovery Boilers

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Fly Ash

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Soot
Extinction
Coefficients
C_2H_2,C_2H_4/O_2
Measurements

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Soot
Nanoparticles
C_2H_4/Air
Below Soot Limit
Absorption Spectra

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PAH,Soot
Aromatic Content
Fingerprint
C_2H_4/O_2
Optical Methods

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Soot Particles
Analysis
C_2H_4,C_3H_8/O_2
PAH Content

(83548) LII Vaporization, Flow Tagging Tracker Method

Soot Velocities

(83840) Aerosols, FT Visible and Infrared Spectra, 0.4-13.9 μm, Size Effects

H_2SO_4,aq

24. NUCLEATION/COAGULATION/CLUSTERS

(See also Section 22 for Nucleation and Growth of Particles)

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(83406)	Biomass Fuels, FBC, Bed Ash, Characteristics	Bed Agglomeration
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(83825)	Infrared Spectrum, Jet Cooled, Diode Lasers, Isomers	$(CO)_2$
(84186)	Thermodynamic Stabilities, C/H/O/Ar, C/H/O/F/Ar, Calculations	C_{60}, C_{70}
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(84151) P.E. Surface, Bound States, Energy Levels, Calculations — NO.Ar

(83852) Photoelectron Spectra, Structure, Frequencies, Contradictions — $(NO)_2, (NO)_2^+$

(84031) Product $N_2(J=74)$ Kinetic Energy, Cluster Effects, m=1-3 — $N_2O(H_2O)_m + h\nu$; $N_2O + h\nu$

(84086) Reaction Dynamics, Channels, Energies, Cluster Effects — $N_2O_5 + nH_2O$

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25. FLAME/CHEMILUMINESCENT SPECTROSCOPY

(83489) Jet Flame Modeling — Radiation Flux

(83865) Chemiluminescence, $B(^2D) + H_2$, Reaction Dynamics — BH(b-a;A-X)

(83869) Chemiluminescence, $Ca(^3P, ^1D) + CH_3I$, CD_3I, Quenching Cross Sections — CaI(C,B,A-X)

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(See also Section 43 for Energy Levels and Theoretically Calculated Spectral Constants, and Section 44 for Vibrational Frequencies and Constants)

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(84180)	PFI-PEPICO Fragmentation Spectrum, CH_3^+ Dissociation Threshold, $D_0(CH_4, CH_4^+)$	CH_4
(83932)	Absorption Spectrum, 8.1 μm Laser, Sensitivities	CH_4, ν_4 $^{13}CH_4, CH_3D$
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N_2O
Overtone
Spectra
Monograph

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CD_2CFO(B-X)
LIF Spectrum
Frequency
Assignments
Radiative Lifetime
$CH_3CFO+h\nu$
Quantum Yield

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CF_3CH_3 ,ν_2 ,ν_8
$\nu_4+\nu_5$,$\nu_6+\nu_9$
FTIR Spectra
Frequencies

(83996) Ultraviolet, Infrared Spectra, Cross Sections, Atmospheric Lifetimes
$(CHF_2)_2O$
$(CF_3CH_2)_2O$
CF_3OCHF_2

(83936) Overtone Spectra, Frequency Modulation, Cavity Enhanced Method, Sensitivities
C_2H_2 ,C_2HD

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$C_2H_2^+$(D,C,B,A,X)
C_2H_2 Photoionization
Cross Sections
IPS
Spectral Analysis
Calculations

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$C_2H_3O^-$

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C_2H_4
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RRS Spectra
Frequencies
Calculations

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C_2H_5
IR Spectrum
Rocking Fundamental
Diode Laser
Constants

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Diode Laser
Isomers

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SRL LIF
Field Effects
Decay
Rate Constants

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Photoelectron
Spectra
Methods

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$CH_3CCH(2\text{-}6\nu_{CH})$
Overtone Spectra
Various Ringdown
Intracavity Methods
Assignments
Constants

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c-$C_4H_6F_2$
Rotational
Spectrum
Constants
Structure

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LIF Spectrum
Assignments
Band Origin

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c-C_4H_8O
Rotational
Spectrum
Jet Cooled
Frequencies
Geometry

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$C_6H_2F_4^+(D_2\text{-}D_0)$
Isomers
Fluorescence
Spectra
Frequencies

(84184) Anion Photoelectron Spectra, X=F,Cl,Br, *o-,m-,p*-Isomers, Vibrational Structure, $D(CH_3C_6H_4X)$

$CH_2C_6H_4X^-$

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27. EXCITED STATE LIFETIMES/QUENCHING

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(84168) Vibrational Relaxation, Rate Constants, Measurements | Bi_2(A,v=1-4)+Rg

(83820) Radiative Lifetime, LIF (B-X) Spectrum, Frequency Assignments | CD_2CFO(B)

(84143) Radiative Lifetime, Ground State P.E. Functions, Energy Levels, Spectral Constants, Calculations | C_2O^-(A)

(84128) Lifetime, fs 2-Photon Ionization/PES Spectroscopy | $C_6H_5OH(S_2)$

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(84072) Cl Exchange Probabilities, Spin-Orbit Effect, Dynamics, Calculations | Cl($^2P_{1/2,3/2}$)+HCl

(83988) Relative Reactivities, Spin-Orbit Effect, Mapping Method | Cl($^2P_{1/2,3/2}$)+H_2

(84074) Reaction Dynamics, P.E. Surfaces, Energies, Transition States | Co^{*+},Co^++H_2O Cu^{*+},Cu^++H_2O Ni^{*+},Ni^++H_2O

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(83989) Crossed Jets, Cross Sections, Spin-Orbit Effect, HF(v=3,J) Product Rotational Distributions | F($^2P_{1/2,3/2}$)+H_2

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Fe^+
Radiative
Lifetimes
Measurements

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Fe^+,W^+
Radiative
Lifetimes
Ion Trap
Technique

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$He(2^3S)+CH_3CN$
Penning Ionization
Product Ion
(C,B,A,X) States
Cross Sections
Calculations

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$He(2^3S)+GeCl_4$
$He(2^3S)+SiCl_4$
Ion Fragment
Emission
Cross Sections
Mechanisms

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$He(2^3S)+HNCO$
$He(2^3S)+HNCS$
Penning Ionization
PES Spectra
Ionic State
Energies,IPs

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$He(2^{1,3}S)+Rg$
Penning Ionization
Rg=Ar,Kr,Xe
Cross Sections
Energy
Dependences
Measurements

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Ho,Ho^+
Radiative
Lifetimes
81,37 Levels
Measurements

83878. Finch, C.D., R. Parthasarathy, S.B. Hill and F.B. Dunning, "Nondissociative Low-Energy Electron Attachment to *c*-C_7F_{14} and C_6F_6: Intermediate Lifetimes," *J. Chem. Phys.* 111, 7316-7320 (1999).

$K(np)+C_6F_6$
$K(np)+c\text{-}C_7F_{14}$
Electron Exchange
$C_6F_6^-$,$c\text{-}C_7F_{14}^-$
Ion Lifetimes

(84081)	Reaction Dynamics, LiH + H Products, P.E. Surfaces, Channels, Energies	$Li^*(3s,2p) + H_2$
(84172)	v,J Relaxation, Angular Momentum Model Application	$Li_2(A,v,J) + Ne$
(83844)	Rate Constants, LiRg($3^2\Sigma^+$) Formation, Rg = Ar,Kr,Xe, P.E. Curves, ($3^2\Sigma^+$-$1^2\Sigma^+$) Emission Spectra	$Li_2(C) + Rg$
83879.	Herron, J.T., "Evaluated Chemical Kinetics Data for Reactions of $N(^2D)$, $N(^2P)$ and $N_2(A^3\Sigma_u^+)$ in the Gas Phase," *J. Phys. Chem. Ref. Data* 28, 1453-1483 (1999).	$N(^2P,^2D),N_2(A)$ Reaction Rate Constants Evaluation
(84082)	Reaction Dynamics, Pathways, Energies	$N(^2D) + HCN$
83880.	Honvault, P., and J.-M. Launay, "A Quantum Mechanical Study of the Dynamics of the $N(^2D) + H_2 \rightarrow NH + H$ Reaction," *J. Chem. Phys.* 111, 6665-6667 (1999).	$N(^2D) + H_2$ Cross Sections Complex Formation Dynamics
83881.	Casavecchia, P., N. Balucani, M. Alagia, L. Cartechini and G.G. Volpi, "Reactive Scattering of Oxygen and Nitrogen Atoms," *Acc. Chem. Res.* 32, 503-511 (1999).	$N(^2D),O(^1D) + H_2$ $O(^1D,^3P) + CH_3I,H_2S$ Crossed Beam Dynamics Overview
83882.	Dilecce, G., and S. De Benedictis, "Experimental Studies on Elementary Kinetics in N_2/O_2 Pulsed Discharges," *Plasma Sources Sci. Technol.* 8, 266-278 (1999).	$N_2(A,v=2\text{-}7) + M$ Quenching Rate Constants $M = NO,O,O_2$ $N_2;N_2/O_2$ Discharge LIF,NO,$N_2(A)$ 2-Photon LIF,O
83883.	Buijsse, B., and W.J. van der Zande, "Photo-predissociation of the $N_2(e^1\Pi_u)$ State in the Presence of a Magnetic Field," *Faraday Discuss. Chem. Soc.* 108, 271-286 (1997).	$N_2(e)$ Predissociation Rotational Lifetimes
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(84087)	OH(v,J) Product Distributions, Reaction Dynamics, P.E. Surface, Calculations, Data Comparisons	$O(^1D) + CH_4$

83885.	Hsu, Y.-T., K. Liu, L.A. Pederson and G.C. Schatz, "Reaction Dynamics of $O(^1D)+HD$. I. The Insertion Pathway," *J. Chem. Phys.* 111, 7921-7930 (1999).	$O(^1D)+HD$ Crossed Beam Product Channels Branching Ratio Cross Sections
83886.	Hsu, Y.-T., K. Liu, L.A. Pederson and G.C. Schatz, "Reaction Dynamics of $O(^1D)+HD$. II. Effects of Excited Surfaces," *J. Chem. Phys.* 111, 7931-7944 (1999).	$O(^1D)+HD$ Cross Beam Measurements Model Inadequacies
(84088)	Reaction Dynamics, Probabilities, Calculations, Data Comparisons	$O(^1D)+HD$
(84091)	Reaction Dynamics, Wavepacket Method, P.E. Surfaces, Probabilities, Product States	$O(^1D)+H_2$,HD
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(84089)	Reaction Dynamics, P.E. Surfaces, Adequacies, Comparisons	$O(^1D)+H_2$
(84090)	Reaction Dynamics, Nonadiabatic Role, Probabilities, Calculations	$O(^1D)+H_2$
83888.	Takahara, A., A. Tezaki and H. Matsui, "Production of SiO and $Si(^3P)$ Atom in the Reaction of Silane with $O(^1D)$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 11315-11320 (1999).	$O(^1D)+SiH_4$ $SiO(v=0\text{-}8)$,Si Product Monitoring Si Branching Ratio $O(^1D)+N_2O,SiH_4$ $Si+N_2O,SiH_4$ Rate Constants
83889.	Yarkony, D.R., "Substituent Effects and the Noncrossing Rule: The Importance of Reduced Symmetry Subspaces. I. The Quenching of $OH(A^2\Sigma^+)$ by H_2," *J. Chem. Phys.* 111, 6661-6664 (1999).	$OH(A)+H_2$ Quenching Dynamics Conical Intersection Role
(83858)	Lifetimes, Three Electronic Spectral Systems, LIF, Low-lying States	RhN
83890.	Parks, H.V., and S.R. Leone, "Alignment and Orientation Effects in Sr Energy Pooling," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 10042-10048 (1999).	$Sr(^3P_1)+Sr(^3P_1)$ Energy Pooling Cross Sections Orientation Effects
83891.	Hirano, I., J. Yoda, F.-L. Hong, K. Okumura and A. Onae, "Collisional Quenching Rates by He, N_2 and CH_4 for the $4D_{3/2}$ State in Sr^+," *Jpn. J. Appl. Phys.* 38, 3747-3748 (1999).	$Sr^+(4^2D_{3/2})+M$ $M=CH_4$,He,N_2 Quenching Rate Constants

28. FRANCK-CONDON FACTORS/TRANSITION PROBABILITIES

(See also Section 27 for Lifetimes and Transition Probabilities)

(84139)	F.C. Factors, *r*-Centroids, D_0 , Constructed P.E. Curves	AlO(D,B-X) BN(A-X) CrO,ScO,YO(B-X) SiO(E-X)
83892.	Wujec, T., A. Baclawski, A. Golly and I. Ksiazek, "Studies of the Bromine Spectrum and Determination of Transition Probabilities for Br and Br^+ Lines," *Acta Phys. Pol. A* 96, 333-340 (1999).	Br,Br^+ Transition Probabilities 5,14 Wavelengths Measurements
83893.	Kleine, D., S. Stry, J. Lauterbach, K. Kleinermanns and P. Hering, "Measurement of the Absolute Intensity of the Fifth CH Stretching Overtone of Benzene Using Cavity Ringdown Spectroscopy," *Chem. Phys. Lett.* 312, 185-190 (1999).	$C_6H_6(6\nu_{CH})$ Overtone Oscillator Strength Cavity Ringdown Absorption
(83562)	Oscillator Strengths, Excitation Energies, Calculations	$C_{10}H_8^+$,$C_{14}H_{10}^+$ $C_{16}H_{10}^+$,$C_{20}H_{12}^+$
(84144)	Transition Probabilities, P.E. Surfaces, Vibrational Energy Levels, Calculations	HOCl,HClO
83894.	Abgrall, H., E. Roueff and I. Drira, "Total Transition Probability and Spontaneous Radiative Dissociation of B, C, B′ and D States of Molecular Hydrogen," *Astron. Astrophys., Suppl. Ser.* 141, 297-300 (2000).	H_2(D,B′,C,B) Radiative Transition Probabilities Calculations
83895.	Luque, J., and D.R. Crosley, "Transition Probabilities and Electronic Transition Moments of the ($A^2\Sigma^+$-$X^2\Pi$) and ($D^2\Sigma^+$-$X^2\Pi$) Systems of Nitric Oxide," *J. Chem. Phys.* 111, 7405-7415 (1999).	NO(D,A-X) Transition Probabilities Moments LIF Measurements 2-Photon Cross Sections
83896.	Fischer, C.F., and X. He, "Transition Energies and Transition Rates for the ($2p^4(^3P)3p$-$2p^4(^3P)3d$) Transitions in Ne^+," *Can. J. Phys.* 77, 177-195 (1999).	Ne^+(3d-3p) Transition Probabilities Calculations
83897.	Horodecki, P., J. Kwela and J.E. Sienkiewicz, "Transition Probabilities of Forbidden Lines in Pb," *Eur. Phys. J. D* 6, 435-440 (1999).	Pb Forbidden Transition Probabilities Calculations

83898. Luke, T.M., "Transition Rates in Singly Ionized Titanium," *Can. J. Phys.* 77, 571-583 (1999).

Ti^+
Transition Probabilities
Low-lying States
Calculations

29. LINESHAPES/STRENGTHS

(84026) Doppler Profiles, CN Product Velocities, ICN + hν Dynamics, D(ICN)

CN(A-X)

83899. Kshirsagar, R.J., L.P. Giver and C. Chackerian Jr., "Rovibrational Intensities of the $(00^03)\leftarrow(10^00)$ Dyad Absorption Bands of $^{12}C^{16}O_2$," *J. Mol. Spectrosc.* 199, 230-235 (2000).

CO_2(003-100)
FT Absorption Spectrum
Bandstrength
Line Intensities

(83836) Infrared Spectrum, Line Positions and Intensities, Tropospheric Application

HCOOH,ν_6

83900. Fono, L., D.J. Donaldson, R.J. Proos and B.R. Henry, "OH Overtone Spectra and Intensities of Pernitric Acid," *Chem. Phys. Lett.* 311, 131-138 (1999).

HNO_3,$3\nu_{OH}$
HNO_4,$3\nu_{OH}$
Absorption
Band Intensities

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NO_2,ν_3
Rg Broadening Coefficients
Lineshifts
Measurements

(83849) Intensities, Absorption Spectrum, ≤22000 cm^{-1}, A/X Conical Intersection, Calculations

NO_2

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OH(A-X)
DFWM
Spectral Lineshapes
C_3H_8/Air

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O_2,1.27 μm
Collision Induced Continuum
Band Strengths
Measurements

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O_2(a)
Broadening Coefficients
Measurements

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O_2(b-X)
Line/Band
Intensities
Positions
Broadening
Coefficients

30. ANALYSIS/MONITORING TECHNIQUES

(See also Section 32 for Mapping and Tomographic Methods)

(84124) ps Pump/Probe, Rate Equation Analyses, Formalism

Laser Diagnostics

83906. Schafer, K., J. Heland, D.H. Lister, C.W. Wilson, R.J. Howes, R.S. Falk, E. Lindermeir, M. Birk, G. Wagner, P. Haschberger, M. Bernard, O. Legras, P. Wiesen, R. Kurtenbach, K.J. Brockmann, V. Kriesche, M. Hilton, G. Bishop, R. Clarke, J. Workman, M. Caola, R. Geatches, R. Burrows, J.D. Black, P. Herve and J. Vally, "Nonintrusive Optical Measurements of Aircraft Engine Exhaust Emissions and Comparison with Standard Intrusive Techniques," *Appl. Opt.* 39, 441-455 (2000).

Nonintrusive
Intrusive
Monitoring Methods
CO,CO_2 ,UHC
Soot
Comparisons
Aircraft Emissions

(83630) Monitoring Intercomparisons, 29 Groups, Atmospheric Measurement Reliability

Nonmethane
Hydrocarbons

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Analysis
Mass Spectrometers
Atmospheric
Monitors
40 Years
Experience

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Molecular Beam
Mass Analyzer
Gas Chromatography
Complementary
Monitors
Low Pressure Flames

(83558) As, Cu, Sb, Se Detection Sensitivities, C_2H_2 /O_2 , Air Flames

Laser Enhanced
Ionization

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Quadrupole
Mass Analyzer
CH_3
Ions
CH_4 Discharge
Monitor

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Mass Analysis
Radicals
CH_3,CF_3,CF_2H
CH_2F,C_2F_5,F
Telluride
Conversion Method

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fs MPI/
Mass Analysis
Supersonic Jet
Aromatic
Hydrocarbon Monitor

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REMPI
$C_6H_5CH_3$
Gasoline Vapor
Fiber Optic
Probe

(83687) Biomass Fires, Trace Gas Emissions, Measurements

FTIR

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FTIR
CO,CO_2,CH_4
C_2H_2,C_2H_4,C_2H_6
NO,N_2O
Spectral Emission
Flame Monitor

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Atomic Emission
Trace Metals
Hg
Smoke Stacks
Discharge Method
O_2 Effects

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Emission
^{15}N Analysis
Discharge Method
N_2(C-B),(2,0)
Interferences

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IR Absorption/
Emission
T,CO_2 Profiles
Monitoring
Method
C_3H_8/Air

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Atomic Emission
ICP/
Microwave Discharge
Tandem Source
Analysis

83918. Lachas, H., R. Richaud, K.E. Jarvis, A.A. Herod, D.R. Dugwell and R. Kandiyoti, "Determination of 17 Trace Elements in Coal and Ash Reference Materials by ICP-MS Applied to Milligram Sample Sizes," *Analyst* 124, 177-184 (1999).

ICP/MS
Ash,Coal
Trace Element
Analysis

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Laser Induced
Breakdown
Spectroscopy
Atomic Analysis

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Laser Induced
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Spectral Analysis
Trace Metals
Aerosols
Review

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Laser Induced
Breakdown Spectra
Trace Metals
Analysis Method

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Laser Induced
Breakdown Spectra
Trace Metals
Monitor

(83452) Particles, Atomic Analysis, Coal Fired MHD

Laser Induced
Breakdown Spectra

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Laser Induced
Breakdown Spectra
Steel Components
C,Cr,Ni,Si
Monitor

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Atomic Absorption
Graphite Furnace
Practical Guide
Monograph

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Atomic Absorption
Heated Furnace
Liquid Jet
Injection
Sensitivities

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83929.	Peterson, K.A., and D.B. Oh, "High Sensitivity Detection of CH Radicals in Flames by Use of a Diode Laser Based Near-Ultraviolet Light Source," *Opt. Lett.* 24, 667-669 (1999).	Absorption CH Wavelength Modulation Diode Laser CH_4,C_2H_4/Air Monitor
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83931.	Ropcke, J., L. Mechold, M. Kaning, W.Y. Fan and P.B. Davies, "Tunable Diode Laser Diagnostic Studies of H_2/Ar/O_2 Microwave Plasmas Containing Methane or Methanol," *Plasma Chem. Plasma Process.* 19, 395-419 (1999).	Absorption Diode Laser CH_3,Stable Species Discharged H_2/O_2/Ar/M M = CH_4,CH_3OH
83932.	Kosterev, A.A., R.F. Curl, F.K. Tittel, C. Gmachl, F. Capasso, D.L. Sivco, J.N. Baillargeon, A.L. Hutchinson and A.Y. Cho, "Methane Concentration and Isotopic Composition Measurements with a Mid-Infrared Quantum Cascade Laser," *Opt. Lett.* 24, 1762-1764 (1999).	Absorption CH_4,ν_4 $^{13}CH_4$,CH_3D 8.1 μm Laser Sensitivities
(84113)	CH_4 Detector, 3.3 μm, 3.5 mW Laser Fabrication	Absorption Diode Laser

(83479) CH_4, CO, C_2H_2, H_2O Pulse Combustor Monitor, Closed Loop Controller — Absorption; Diode Laser

83933. Durry, G., and G. Megie, "Atmospheric CH_4 and H_2O Monitoring with Near-Infrared InGaAs Laser Diodes by Balloonborne Spectrometer for Tropospheric and Stratospheric in Situ Measurements," *Appl. Opt.* 38, 7342-7354 (1999). — Absorption; CH_4,H_2O; Laser Diodes; Atmospheric Measurements

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(83893) $C_6H_6(6\nu_{CH})$ Overtone, Oscillator Strength, Measurement — Absorption; Cavity Ringdown

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(83703) HF Emissions, Enclosed Pan Fires, C_7H_6/Air, $C_3F_6H_2$, C_3F_7H, Ammonium Polyphosphate Additives — Absorption; Diode Laser

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Absorption
H_2O
Laser Diode
Modulation
Methods Compared
Sensitivity

(83685) H_2O, O_2 Monitor, Incineration, Active Controller

Absorption
Diode Laser

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UV Absorption
Zeeman Modulated
Hg
Flue Gas Emissions
$HgCl_2$ Reducer

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DIAL
NO
Remote
Monitor

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Absorption
NO
NDIR Detector
Auto Roadside
Monitor

(83649) Monitoring Comparisons, Reliabilities

DOAS/ESR
NO_3

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Absorption
Pulsed Xe Lamp
T,OH,NO
Propellant
Combustion
CCD Detector

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Absorption
O_2 ,763 nm
Cavity Enhanced
Minimum
Detectability
Monitor

(84114) O_2(a), H_2O Monitoring, Iodine/Oxygen Chemical Laser

Absorption
Diode Laser

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DOAS
O_3
279-289 nm
Unidentified
Interfering
Absorber

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DIAL
SO_2
Multiwavelength
Improved
Accuracies

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Absorption
YO
Xe Lamp
Y_2O_3 Ablation
Plume

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Laser Excited
Atomic
Fluorescence
Ablation
Monitor

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PLIF,CH(A-X)
Optimization
Background Filters
Monitor

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LIF
C_2
Formation
C_4F_8 Discharge
Wall Mechanism
Monitoring

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Fragmentation
LIF
$C_6H_4(NO_2)_2$
Monitor NO
Sensitivity

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Laser
Photofragmentation
H_2O,NH_3,NO_2
Nitro-Explosives
H_2SO_4,SO_2
Fragment Monitoring

(83445) TNT, PETN, RDX, Product NO, NO_2 Detection

Photofragmentation
LIF,REMPI

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83954.	Chadwick, B.L., D. Charlston-Goch, A. Campisi and R.J.S. Morrison, "Flame Front Observation of Ammonia Decomposition and Oxidation Using 193 nm Two-Photon Photolysis and Photofragment Fluorescence," *Appl. Spectrosc.* 53, 1222-1225 (1999).	2-Photon Dissociation Fragment Fluorescence NH_3 Detection CH_4/NH_3/Air Flames
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83956.	Thornton, J.A., P.J. Wooldridge and R.C. Cohen, "Atmospheric NO_2: In Situ Laser Induced Fluorescence Detection at Parts per Trillion Mixing Ratios," *Anal. Chem.* 72, 528-539 (2000).	LIF NO_2 Time Gated High Sensitivity Method
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83958.	Matousek, P., M. Towrie, A. Stanley and A.W. Parker, "Efficient Rejection of Fluorescence from Raman Spectra Using Picosecond Kerr Gating," *Appl. Spectrosc.* 53, 1485-1489 (1999).	Raman Spectra ps Kerr Gate Fluorescence Rejection Method
(84098)	Monitor, CH_4 Microwave Discharge, Temperature, Densities	CARS CH_3,CH_4,H_2
83959.	Lang, T., K.-L. Kompa and M. Motzkus, "Femtosecond CARS on H_2," *Chem. Phys. Lett.* 310, 65-72 (1999).	fs CARS H_2 J Level Monitor

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CARS
N_2(v),NO
Measurements
N_2/O_2/NO
Discharges
NO Control

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(See also Section 34 for Flame Species Profiles)

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Species Profiles
$C_2H_6/C_3HF_7/H_2$/Air
Flame Inhibition
Mechanisms

32. MAPPING/TOMOGRAPHIC METHODS

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Tomography
T,Velocities
Flowfield

(83457) Heated Gas Flow Temperatures, Algorithm

IR Emission
Tomography

(83575) Visualization, Flame/Surface Interactions

Laser Sheet
Tomography

(83456) Temperatures, Multijet Turbulent Flame

Speckle Tomography

(84024) Product Angular Momentum Polarization, CH_3I, OCS, Cl_2, N_2O, O_2, O_3 Photolyses

2-D Ion Imaging

83963. Chandler, D.W., and D.H. Parker, "Velocity Mapping of Multiphoton Excited Molecules," *Adv. Photochem.* 25, 59-106 (1999).

2-D Mapping
Velocities
MPD Fragments
D_2,O_2
Ion Imaging

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PLIF,NO
T,Pressure
Measurements
Mach 3
Flowfield

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PLIF,NO
Hypersonic Flows
Measurements
CFD Modeling
Comparisons

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2-D Raman Imaging
N_2,O_2
Supersonic
Nozzle Flow

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PLIF,OH
Rayleigh
Scattering
Turbulent
Jet Flames
Structure

83968. Yamamoto, T., N. Kobayashi and N. Arai, "Simultaneous Measurements of Planar Profiles of OH Radicals and Temperature in the Field of Pressurized Methane/Air Combustion by the PLIF," pp. 503-510 in *Proceedings of the 1997 International Joint Power Generation Conference. Volume 1. Environmental Control/Fuels and Combustion Technologies/Nuclear Engineering*, A. Sanyal, A. Gupta and J. Veilleux, eds., 77 Papers Presented in Denver CO, November 1997, ASME Publication EC-Vol. 5, 678 pp., The American Society of Mechanical Engineers, New York (1997).

2-D Mapping
T,PLIF OH
High Pressure
CH_4/Air

33. OPTOGALVANIC/OPTOACOUSTIC METHODS

34. FLAME KINETIC MODELING

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Kinetic Modeling
Scheme Reduction
Optimization
$CH_4/O_2/N_2$
H_2/O_2
O_3
Testing

(83979) Kinetic Modeling, Sensitivity Coefficient Analysis, New Direct Method

$CH_2O/CO/O_2$

(83737) Kinetic Modeling, NO Formation, Counterflow Flames, LIF Measurements

CH_4/Air

83970. Werner, J.H., and T.A. Cool, "The Kinetics of the Combustion of Trichloroethylene for Low Cl/H Ratios," *Combust. Flame* 120, 125-142 (2000).

Kinetic Modeling
$CH_4/O_2/Ar$
C_2HCl_3 Additive
Species Profiles
Major Channels

83971. Williams, B.A., D.M. L'Esperance and J.W. Fleming, "Intermediate Species Profiles in Low Pressure Methane/Oxygen Flames Inhibited by 2-H Heptafluoropropane: Comparison of Experimental Data with Kinetic Modeling," *Combust. Flame* 120, 160-172 (2000).

Kinetic Modeling
$CH_4/C_3HF_7/O_2$
Species Profiles
Inhibition
Data Comparisons

83972. Hidaka, Y., K. Sato, H. Hoshikawa, T. Nishimori, R. Takahashi, H. Tanaka, K. Inami and N. Ito, "Shock Tube and Modeling Study of Ethane Pyrolysis and Oxidation," *Combust. Flame* 120, 245-264 (2000).
Kinetic Modeling
C_2H_6
C_2H_6/O_2
Shock Tube Measurements
Sensitivity Analysis

83973. Reisel, J.R., "Modeling of Nitric Oxide Formation in High Pressure Premixed Laminar Ethane Flames," *Combust. Flame* 120, 233-241 (2000).
Kinetic Modeling
$C_2H_6/O_2/N_2$
NO Formation
High Pressures
Revised Mechanism

83974. Taconnet, S., Y. Simon, G. Scacchi and F. Baronnet, "Experimental and Modeling Study of *neo*- and *iso*-Pentane Oxidation," *Can. J. Chem.* 77, 1177-1190 (1999).
Kinetic Modeling
neo-,i-C_5H_{12}/O_2
Stirred Reactor
873 K
Auto-ignition

35. PYROLYSIS KINETICS/STUDIES

(83762) Soot Formation, Induction Period, Number Density
CCl_4 Pyrolysis
CCl_4/CH_4

(83764) Soot Formation, PAH Growth, Measurements, Modeling
C_2H_2, C_6H_6
Pyrolysis

83975. Roscoe, J.M., A.R. Bossard and M.H. Back, "A Kinetic Modeling Study of Ethylene Pyrolysis," *Can. J. Chem.* 78, 16-25 (2000).
Pyrolysis
C_2H_4
Kinetic Model

(83772) Soot Formation, $Fe(CO)_5$ Effects, Shock Tube Measurements
C_2H_4 Pyrolysis

83976. Pavlov, A.N., V.N. Grebennikov, L.D. Nazina, G.M. Nazin and G.B. Manelis, "Thermal Decomposition of Ammonium Dinitramide and Mechanism of Anomalous Decay of Dinitramide Salts," *Russ. Chem. Bull.* 48, 50-54 (1999).
Pyrolysis
$NH_4N(NO_2)_2$
Mechanism

36. KINETIC MODELING/SENSITIVITIES/RATE CONSTANTS

(See also Section 15 for Ion Reaction Rate Constants, Section 27 for Excited State Rate Constants, Section 39 for Unimolecular Rate Constants, Section 40 for Theoretically Calculated Values and Section 45 for Energy Relaxation Rate Constants)

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Rate Constants
Photochemistry
Halogen Species
Atmospheric Processes
Critical Evaluation

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Kinetic Modeling
New Solver Approach
3-D Atmospheric Chemistry Application

(83617) Atmospheric Chemistry, Equivalent Kinetic Operator, New Efficient Approach

Kinetic/Transport 3-D Models

(83618) Tropospheric Photochemical Model, Species Densities, Data Comparisons

Kinetic/Transport Model

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Kinetic Modeling
Sensitivity Coefficient Analysis
New Direct Method
$CH_2O/CO/O_2$
$(CH_3)_2S/O_2+h\nu$

83980. Naulin, C., and M. Costes, "Crossed Beam Study of the $Al(^2P_{1/2,3/2})+O_2(X^3\Sigma_g^-)\rightarrow AlO(X^2\Sigma^+)+O(^3P_J)$ Reaction at Low and Very Low Kinetic Energies," *Chem. Phys. Lett.* 310, 231-239 (1999).

$Al(^2P_J)+O_2$
Rate Constants
Crossed Beams
Spin-Orbit Effects
$D_0(AlO)$

83981. Lam, S.K., C.-E. Zheng, D. Lo, A Dem'yanov and A.P. Napartovich, "Kinetics of Ar_2* in High Pressure Pure Argon," *J. Phys. D. Appl. Phys.* 33, 242-251 (2000).

Ar_2* Reactions
Kinetic Modeling
Ar Discharge

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CF_2+H
CF_2+O
Rate Constants
T Dependences
P Independence
Shock Tube

83983. Ibragimova, L.B., G.D. Smekhov and O.P. Shatalov, "Dissociation Rate Constants of Diatomic Molecules under Thermal Equilibrium Conditions," *Fluid Dyn., Russia* 34, 153-157 (1999).

CN,CO,C_2
NO,N_2,O_2
Thermal Dissociation
Rate Constants
300-40000 K
Assessments

(83975) Pyrolysis, Kinetic Model

C_2H_4

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C_3H_6, i-$C_4H_8+O_3$
$C_5H_8+O_3$
OH Product Yields
Rate Constants
Mechanisms

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$C_6H_5+C_6H_6$
$C_6H_5+C_6D_6$
Rate Constants
T Dependences
Measurements

83986. Taatjes, C.A., L.K. Christensen, M.D. Hurley and T.J. Wallington, "Absolute and Site-Specific Abstraction Rate Coefficients for Reactions of Cl with CH_3CH_2OH, CH_3CD_2OH and CD_3CH_2OH between 295 and 600 K," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 9805-9814 (1999).

$Cl+C_2H_5OH$
$Cl+CH_3CD_2OH$
$Cl+CD_3CH_2OH$
Rate Constants
Site Selectivity
HCl(v=0,1) Product

83987. Manke II, G.C., T.L. Henshaw, T.J. Madden and G.D. Hager, "Temperature Dependence of the $Cl+HN_3$ Reaction from 300 to 480 K," *Chem. Phys. Lett.* 310, 111-120 (1999).

$Cl+HN_3$
Rate Constants
T Dependence

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$Cl(^2P_{1/2,3/2})+H_2$
Reactivities
$(^2P_{1/2})$ Enhancements
Mapping Method

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$F(^2P_{1/2,3/2})+H_2$
Crossed Jets
Cross Sections
HF(v=3,J)
Product
Rotational
$F(^2P_{1/2})$ Role

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Li+NO+Ar
Na+NO+Ar
K+NO+Ar
Rate Constants
RRKM Modeling
D(NaNO,KNO)

83991. Vinckier, C., J. Helaers, P. Christiaens and J. Remeysen, "Kinetic Investigation of the Reactions of $Mg(^1S)$, $Ca(^1S)$ and $Sr(^1S)$ Atoms with NO_2 Over the Temperature Ranges 303-836, 303-916 and 303-986 K, Respectively," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 11321-11327 (1999).

$Mg+NO_2$
$Ca,Sr+NO_2$
Rate Constants
T Dependences

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Mo+Y
Mo_2+Y
Rate Constants
$Y=CO,C_2H_4,H_2,$
NH_3,NO,O_2,SF_6
$Mo(CO)_6$ UV MPD

(83879) Reaction Rate Constants, Evaluation

$N(^2P,^2D),N_2(A)$

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$NCS+C_2H_2,O_2$

Phys. Chem. A. Mol., Spectrosc., Kinetics 103, 11340-11344 (1999). — $NCS + NO,NO_2$ / Rate Constants / T,P Dependences

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(83888) Rate Constants, Measurements — $Si + N_2O,SiH_4$

37. PHOTOLYSIS/MPD

(See also Section 38 for Photolytic Product Distributions)

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(83820)	CH_2CFO Radical Quantum Yield, 193 nm Photolysis	CH_3CFO + hν
(84044)	CH_3CO Product Formation, 193 nm Photolyses, non-RRKM Behavior	CH_3COOH + hν CH_3COCN + hν
84010.	Xu, K., G. Amaral and J. Zhang, "Photodissociation Dynamics of Ethanol at 193.3 nm: The H-Atom Channel and Ethoxy Vibrational Distribution," *J. Chem. Phys.* 111, 6271-6282 (1999).	C_2H_5OH + hν C_2H_5OD + hν Channels Product Energies $D(C_2H_5OH,C_2H_5OD)$
(83979)	Kinetic Modeling, Sensitivity Coefficient Analysis, New Direct Method	$(CH_3)_2S/O_2$ + hν
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84012.	Forde, N.R., T.L. Myers and L.J. Butler, "Chemical Reaction Dynamics when the Born-Oppenheimer Approximation Fails: Understanding Which Changes in the Electronic Wavefunction Might be Restricted," *Faraday Discuss. Chem. Soc.* 108, 221-242 (1997).	$Br(CH_2)_2COCl$ + hν $HCON(CH_3)_2$ + hν Reaction Dynamics Nonadiabatic Descriptions
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84014.	Suter, H.U., J.R. Huber and T.-K. Ha, "Photodissociation of Carbonyl Cyanide $CO(CN)_2$: An ab Initio Calculation Study," *Chem. Phys. Lett.* 311, 474-478 (1999).	$CO(CN)_2$ + hν Channels Dynamics Calculations

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fs MPD/MPI
$Fe(CO)_5$
Laser Control
Pulse Shaper
Method

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HNCO + hν
Photodissociation
Dynamics
Channels
Product Energies
Calculations

(84129) Dynamics, H(n = 3) Product, (1 + 1′) REMPI Dissociation

$H_2(B)$ + hν

(83992) Mo, Mo_2 Source, Rate Constant Measurements

UV MPD
$Mo(CO)_6$

84017. Lopez-Martens, R.B., T.W. Schmidt and G. Roberts, "Femtosecond Fluorescence Depletion Spectroscopy of NO_2 Multiphoton Dissociation Dynamics," *J. Chem. Phys.* 111, 7183-7186 (1999).

MPD
NO_2
fs Pump/Probe
NO(A,v = 0,1)
Product
Mechanism

84018. Parsons, B.F., S.L. Curry, J.A. Mueller, P.C. Ray and L.J. Butler, "Emission Spectroscopy of Photodissociating N_2O_4 Excited Near 200 nm to the $\pi_{nb,O}\pi^*_{NO2}/n\sigma^*_{N-N}$ Avoided Crossing," *J. Chem. Phys.* 111, 8486-8495 (1999).

N_2O_4 + hν
Product Emission
Frequencies
Mechanism

84019. Chang, X.Y., R. Ehlich, A.J. Hudson, P. Piecuch and J.C. Polanyi, "Dynamics of Harpooning Studied by Transition State Spectroscopy Na···FH," *Faraday Discuss. Chem. Soc.* 108, 411-425 (1997).

Na···FH + hν
Transition State
Photodepletion
Spectrum
Cross Sections

(84122) Laser Control, Optimal Neutral Products Method

NaI + hν

84020. Magnier, S., M. Persico and N. Rahman, "Theoretical Study of Two-Photon Above Threshold Dissociation and Related Processes in Na_2^+ and Li_2^+," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 10691-10698 (1999).

$Na_2^+ + h\nu_1 + h\nu_2$
$Li_2^+ + h\nu_1 + h\nu_2$
2-Photon Above
Threshold
Dissociation
Calculations

(84192) $O(^1D) + O_2(a)$ Product Threshold, VUV LIF, REMPI Imaging, $\Delta H_f(O_3)$

O_3 + hν

84021. Lokhman, V.N., A.N. Petin, E.A. Ryabov and V.S. Letokhov, "Transition Spectra in the Vibrational Quasicontinuum of Polyatomic Molecules. Infrared Multiphoton Absorption in SF_6. I. Experimental Studies," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 11293-11298 (1999).

Infrared
IR MPA
SF_6, ν_3
Pump/Probe
Measurements

84022.	Lokhman, V.N., A.A. Makarov, I.Yu. Petrova, E.A. Ryabov and V.S. Letokhov, "Transition Spectra in the Vibrational Quasicontinuum of Polyatomic Molecules. Infrared Multiphoton Absorption in SF_6. II. Theoretical Simulation and Comparison with Experiment," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 11299-11309 (1999).	IR MPA SF_6 ,ν_3 Simulated Absorption Spectrum
(83784)	Si Nanoparticles, Nucleation, Growth, Raman, LIF Monitoring	IR MPD,SiH_4
(83802)	Photodissociation Products, Branching Ratios, Mass Analysis, n=1-4, m=1-6	$Sr^+(H_2O)_n+h\nu$ $Sr^+(D_2O)_m+h\nu$

38. REACTION PRODUCT-ENERGY DISTRIBUTIONS

(See also Section 37 for Product Distributions)

84023.	Rakitzis, T.P., G.E. Hall, M.L. Costen and R.N. Zare, "Relationship between Bipolar Moments and Molecule-Frame Polarization Parameters in Doppler Photofragment Spectroscopy," *J. Chem. Phys.* 111, 8751-8754 (1999).	Photofragment Doppler Profiles Polarized Photolysis Formalism
84024.	Mo, Y., and T. Suzuki, "Optical Detection of Angular Momentum Polarization and Its Application to Photodissociation Dynamics," *Adv. Multiphoton Process. Spectrosc.* 12, 185-226 (1999).	Product Angular Momentum Polarization CH_3I,OCS,$Cl_2+h\nu$ N_2O,O_2 ,$O_3+h\nu$ 2-D Ion Imaging Method
(83865)	Product Energies, $B(^2D)+H_2$, Chemiluminescence, Reaction Dynamics	BH(b,A)
84025.	Martinez-Haya, B., I. Zapater, P. Quintana, M. Menendez, E. Verdasco, J. Santamaria, L. Banares and F.J. Aoiz, "Photodissociation of Dimethyl Sulfide at 227.5 nm: Resonance-Enhanced Multiphoton Ionization of the Methyl Fragment," *Chem. Phys. Lett.* 311, 159-166 (1999).	CH_3 Product Energies $(CH_3)_2S+h\nu$ REMPI Probe
84026.	Costen, M.L., S.W. North and G.E. Hall, "Vector Signatures of Adiabatic and Diabatic Dynamics in the Photodissociation of ICN," *J. Chem. Phys.* 111, 6735-6749 (1999).	CN Product Velocities (A-X) Doppler Profiles $ICN+h\nu$ Dynamics D(ICN)
84027.	Carter, R.T., A. Hallou and J.R. Huber, "Photodissociation of $ClNO_2$ at 235 nm," *Chem. Phys. Lett.* 310, 166-172 (1999).	$Cl(^2P_{3/2})$ Product Energies Anisotropies $ClNO_2+h\nu$ Dissociative Lifetime

84028.	Ascenzi, D., P.M. Regan and A.J. Orr-Ewing, "The Ultraviolet Photodissociation of DCl: H/D Isotope Effects on the $Cl(^2P)$ Atom Spin-Orbit Branching," *Chem. Phys. Lett.* 310, 477-484 (1999).	$Cl(^2P_{1/2,3/2})$ Product Branching Ratios HCl,DCl + hν Isotope Wavelength Effects
(83986)	$Cl + C_2H_5OH$, CH_3CD_2OH, CD_3CH_2OH Rate Constants, Site Selectivity	HCl(v = 1,0) Product Branching
84029.	Lin, S.-R., and Y.-P. Lee, "Photodissociation of 1,1-Difluoroethene (CH_2CF_2) at 193 nm Monitored with Step-Scan Time-Resolved Fourier Transform Infrared Emission Spectroscopy," *J. Chem. Phys.* 111, 9233-9241 (1999).	HF(v = 1-5),H Product Channels CF_2CH_2 + hν HF,HCl(Added Cl_2) Vibrational Relaxation Rate Constants
(83989)	Product Rotational Distributions, $F(^2P_{1/2,3/2}) + H_2$, Crossed Jets, Cross Sections, Spin-Orbit Effect	HF(v = 3,J)
84030.	Dobeck, L.M., H.M. Lambert, W. Kong, P.J. Pisano and P.L. Houston, "H_2 Production in the 440 nm Photodissociation of Glyoxal," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 10312-10323 (1999).	H_2(v,J) Product Energy Distribution $(CHO)_2$ + hν
(84085)	NH + H Product Energies, Reaction Dynamics, Calculations	H_2(v,J)
84031.	Gandhi, S.R., "Velocity of N_2 upon Dissociation of N_2O in $N_2O(H_2O)_m$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 10713-10718 (1999).	N_2(J = 74) Kinetic Energy N_2O + hν $N_2O(H_2O)_m$ + hν Comparisons
84032.	Lee, S., "Vector Properties of $O(^3P)$ and $O(^1D)$ in OH Photodissociation: Near-Threshold Resonance, Neighboring Resonance and Above-Threshold Behavior," *J. Chem. Phys.* 111, 6407-6412 (1999).	$O(^1D,^3P)$ Product Vector Properties OH + hν Calculations
84033.	Neyer, D.W., A.J.R. Heck, D.W. Chandler, J.M. Teule and M.H.M. Janssen, "Speed-Dependent Alignment and Angular Distributions of $O(^1D_2)$ from the Ultraviolet Photodissociation of N_2O," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 10388-10397 (1999).	$O(^1D)$ Velocity Distributions Alignments N_2O + hν
(84087)	Product Distributions, $O(^1D) + CH_4$, Reaction Dynamics, P.E. Surface, Calculations, Data Comparisons	OH(v,J)

84034. Costen, M.L., G. Hancock and G.A.D. Ritchie, "Dynamics of the Reaction $O(^3P)+H_2S \rightarrow OH+SH$. I. Rotational, Λ Doublet and Fine Structure Distributions in the $OH(v''=1)$ Product," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 10644-10650 (1999).
OH(X,v=1,J)
Product Energy
Distribution
$O+H_2S$
Measurements

84035. Costen, M.L., G. Hancock and G.A.D. Ritchie, "Dynamics of the Reaction $O(^3P)+H_2S \rightarrow OH+SH$. II. State-Resolved Differential Cross Sections and Angular Momentum Correlations," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 10651-10663 (1999).
OH,SH
Product
Scattering
Angular Momentum
$O+H_2S$
Measurements

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$OH^-(v),OD^-(v)$
Product Energies
O^-+D_2
O^-+H_2
Collision Energy
Effects

39. UNIMOLECULAR PROCESSES

(See also Section 36 for Unimolecular Rate Constants)

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Unimolecular
Dissociation
Ions
H_2 Elimination
Energy Release
Review

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Unimolecular
Dissociation
CH_3O+He,N_2
Rate Constants
Tunneling Role
RRKM Analysis

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Unimolecular
Dissociation
CH_3S^+
^{1,3}P.E. Surfaces
RRKM Calculations
Rate Constants

84040. Martinez-Nunez, E., and S.A. Vazquez, "Classical Dynamics Study of the Unimolecular Decomposition of CH_3SH^+," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 9783-9793 (1999).
Unimolecular
Dissociation
CH_3SH^+
Channels
RRKM Calculations
Rate Constants

84041. King, R.A., W.D. Allen, B. Ma and H.F. Schaefer III, "Fragmentation Surface of Triplet Ketene," *Faraday Discuss. Chem. Soc.* 110, 23-50 (1998).

Unimolecular Dissociation
$CH_2CO(a^3A'')$
Triplet Surface
Dynamics

84042. Hoxha, A., R. Locht, A.J. Lorquet, J.C. Lorquet and B. Leyh, "Unimolecular Dynamics from Kinetic Energy Release Distributions. V. How Does the Efficiency of Phase Space Sampling Vary with Internal Energy?," *J. Chem. Phys.* 111, 9259-9266 (1999).

Unimolecular Dissociation
$C_2H_3Br^+$
Product
Energy Release

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Unimolecular Dissociation
CH_2CHNO_2
Channels
Energies

84044. Owrutsky, J.C., and A.P. Baronavski, "Ultrafast Photodissociation Studies of Acetyl Cyanide and Acetic Acid and Unimolecular Decomposition Rates of the Acetyl Radical Products," *J. Chem. Phys.* 111, 7329-7336 (1999).

Unimolecular Dissociation
CH_3CO
RRKM Analysis
$CH_3COOH+h\nu$
$CH_3COCN+h\nu$
Precursors

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Unimolecular Dissociation
$CH_3C(O)OONO_2$
Pathways
ΔH_f(PAN,$CH_3C(O)O_2$)
$\Delta H_f(CH_3C(O)O)$
Calculations

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Unimolecular Reactions
$C_2H_5+O_2$
Multi-well
Multichannel
Master Equation
Analysis

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Unimolecular Dissociation
$(CH_3)_2NNO_2$
Channels
NO_2,HONO
Products
Energies
Dynamics

84048. Fueno, H., and Y. Taniguchi, "Ab Initio Molecular Orbital Study of the Isomerization Reaction Surfaces of C_3 and C_3^-," *Chem. Phys. Lett.* 312, 65-70 (1999).

Isomerization
C_3 ,C_3^-
P.E. Surfaces
Low-lying States
Linear/Bent Structures

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Unimolecular
Photoisomerization
$C_6H_5CHCHC_6H_5$
Rate Constants
CH_4 ,C_2H_6 ,C_3H_8 ,Xe
Bath Gases

84050. Guo, Y., D.L. Thompson and W.H. Miller, "Thermal and Microcanonical Rates of Unimolecular Reactions from an Energy Diffusion Theory Approach," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 10308-10311 (1999).

Unimolecular
Dissociation
RDX
Collision Activation
Limited
Model
Rate Constants

84051. Li, Z., and J.S. Francisco, "A Coupled-Cluster Study of the HOBr→HBrO Transition State," *J. Chem. Phys.* 111, 5780-5782 (1999).

Isomerization
HOBr/HBrO
Energy
Barrier
Calculations

84052. Callegari, A., J. Rebstein, R. Jost and T.R. Rizzo, "State-to-State Unimolecular Reaction Dynamics of HOCl Near the Dissociation Threshold: The Role of Vibrations, Rotations, and IVR Probed by Time and Eigenstate Resolved Spectroscopy," *J. Chem. Phys.* 111, 7359-7368 (1999).

Unimolecular
Dissociation
HOCl
Rates
Overtone
Excitation
OH Product Energies

84053. Goumri, A., J.-D.R. Rocha, D. Laakso, C.E. Smith and P. Marshall, "Characterization of Reaction Pathways on the Potential Energy Surfaces for $H+SO_2$ and $HS+O_2$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 11328-11335 (1999).

Unimolecular
Dissociation
Isomerization
HSO_2 ,HOSO
HOOS
P.E. Surfaces
Barriers
D(HOSO)

84054. Llanio-Trujillo, J.L., J.M.C. Marques and A.J.C. Varandas, "Mode Specificity Study in Unimolecular Dissociation of Nonrotating H_2O, DHO and MuHO Molecules," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 10907-10914 (1999).

Unimolecular
Dissociation
H_2O,DHO,MuHO
Vibrational Mode
Effects
Calculations

84055. Bezel, I., D. Stolyarov and C. Wittig, "Unimolecular Reaction Rate Constants of NO_2 Just Above D_0," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 10268-10273 (1999).

Unimolecular Dissociation
NO_2
17 cm^{-1} Above Threshold
ps Pump/Probe
Rate Constants

84056. Demyanenko, A.V., V. Dribinski, H. Reisler, H. Meyer and C.X.W. Qian, "Product Quantum State Dependent Anisotropies in Photoinitiated Unimolecular Decomposition," *J. Chem. Phys.* 111, 7383-7396 (1999).

Unimolecular Dissociation
$NO_2 + h\nu$
Jet Cooled
NO(v),O
Angular Distributions

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Unimolecular Dissociation
NO_2
Near Threshold
Rate Constants
Pump/Probe Method

40. CHEMICAL DYNAMICS - THEORY

(See also Section 37 for Photodissociation Dynamics)

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Reaction Dynamics
Rate Theory
Recent Theoretical Developments
Overview

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Reaction Dynamics
Hyperspherical Coordinates Approach

84060. Fang, J.-Y., and S. Hammes-Schiffer, "Improvement of the Internal Consistency in Trajectory Surface Hopping," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 9399-9407 (1999).

Reaction Dynamics
Modified Surface Hopping Method

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Reaction Dynamics
Dynamical Tunneling
IVR
2 P.E. Surfaces

84062. Morokuma, K., Q. Cui and Z. Liu, "Potential Energy Surfaces and Their Dynamic Implications," *Faraday Discuss. Chem. Soc.* 110, 71-89 (1998).

Reaction Dynamics
$CH+N_2$
$C_2H_2^+ + CH_4$
P.E. Surfaces
Rates
Calculations

84063. Klippenstein, S.J., and L.B. Harding, "A Direct Transition State Theory Based Study of Methyl Radical Recombination Kinetics," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 9388-9398 (1999).

Reaction Dynamics
CH_3+CH_3+M
TST
Rate Constants
Energy Transfer

84064. Susnow, R.G., A.M. Dean and W.H. Green Jr., "Hydrogen Abstraction Rates via Density Functional Theory," *Chem. Phys. Lett.* 312, 262-268 (1999).

Reaction Dynamics
CH_3+HCHO,C_2H_6
$CH_3+HCOOH$
Rate Constants
DFT Method

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Reaction Dynamics
TS Wavepacket Method
$CN+H_2,D_2$
Rate Constants

84066. Tsuchiya, K., K. Kamiya, H. Shiina and M. Oya, "Computational Studies on the Reactions of N_2O with $O(^3P)$ and CO," *Chem. Lett. Jpn.* 609-610 (1999).

Reaction Dynamics
$CO+N_2O$
$O+N_2O$
Rate Constants
Transition States

84067. Good, D.A., M. Kamboures, R. Santiano and J.S. Francisco, "Atmospheric Oxidation of Fluorinated Ethers, E143a(CF_3OCH_3), E134(CHF_2OCHF_2) and E125(CHF_2OCF_3)," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 9230-9240 (1999).

Reaction Dynamics
CF_3OCH_3/O_2
$(CHF_2)_2O/O_2$
CHF_2OCF_3/O_2
Channels
Energies

84068. Chandra, A.K., and T. Uchimaru, "An ab Initio Investigation of the Reactions of 1,1- and 1,2-Dichloroethane with Hydroxyl Radical," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 10874-10883 (1999).

Reaction Dynamics
$C_2H_4Cl_2+OH$
Structures
Barrier Heights
Rate Constants

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Reaction Dynamics
$C_4H_6^+ + C_2H_4$
Channels
Energetics

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Reaction Dynamics
t-$C_4H_9+O_2$
i-$C_4H_8+HO_2$,OH
Oxidation
Mechanism
RRKM Analysis

84071. Yu, H.-G., and G. Nyman, "Reaction Dynamics of Chlorine Atom with Methane: Dual-Level ab Initio Analytic Potential Energy Surface and Isotope Effects," *J. Chem. Phys.* 111, 6693-6704 (1999).

Reaction Dynamics
$Cl+CH_4$,CD_4
P.E. Surface
Barrier Height
Rate Constants
Tunneling

84072. Schatz, G.C., P. McCabe and J.N.L. Connor, "Quantum Scattering Studies of Spin-Orbit Effects in the $Cl(^2P)+HCl \rightarrow ClH+Cl(^2P)$ Reaction," *Faraday Discuss. Chem. Soc.* 110, 139-157 (1998).

Reaction Dynamics
Cl+HCl
Cl Exchange
Probabilities
$Cl(^2P_{1/2},{}^2P_{3/2})$
Effects

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Reaction Dynamics
$Cl+H_2$
P.E. Surfaces
Resonance States
Calculations

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Reaction Dynamics
Co^+,$Co^{*+}+H_2O$
Ni^+,$Ni^{*+}+H_2O$
Cu^+,$Cu^{*+}+H_2O$
P.E. Surfaces
Energies
Transition States

84075. Castillo, J.F., and D.E. Manolopoulos, "Quantum Mechanical Angular Distributions for the F+HD Reaction," *Faraday Discuss. Chem. Soc.* 110, 119-139 (1998).

Reaction Dynamics
F+HD
P.E. Surface
Probabilities
Calculations

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Reaction Dynamics
F+HD
HF,DF Channels
Cross Sections
Isotopic Preferences

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Reaction Dynamics
GeH_4+H
GeD_4+H
P.E. Surface
Construction
Performance

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Reaction Dynamics
Reactant/Product
Decoupling
Method
$H+H_2$

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H_3, D_3
Predissociation
Dynamics
Rydberg/
Ground State
Interactions
Calculations

(84146) Reaction Dynamics, Channels, H_3O^+ P.E. Surface, Rate Constants, Calculations

$H_3^++O/H_2O^++H/$
OH^++H_2

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Reaction Dynamics
$Li+HF$
Probabilities
Angle of Attack
Effects

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Reaction Dynamics
$Li^*(3s,2p)+H_2$
$LiH+H$
P.E. Surfaces
Channels
Energies

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Reaction Dynamics
$N(^2D)+HCN$
Pathways
Energies

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N^++CH_3
$N+CH_3^+$
$CH_2N^++e^-$
HCN/HNC Product
Mechanism

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$NH+CH_nF_{4-n}$
$NH+CD_nF_{4-n}$
Rate Constants
Energy Barriers
Calculations

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$NH+H$
$H_2(v,J)$ Product
Energies
Calculations

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Reaction Dynamics
$N_2O_5+nH_2O$
Channels
Energies
Cluster Effects

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Reaction Dynamics
$O(^1D)+CH_4$
P.E. Surface
OH(v,J) Product
Distributions
Calculations
Data Comparisons

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Reaction Dynamics
$O(^1D)+HD$
Probabilities
Calculations
Data Comparisons

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Reaction Dynamics
$O(^1D)+H_2$
P.E. Surfaces
Adequacies
Comparisons

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Reaction Dynamics
$O(^1D)+H_2$
Nonadiabatic Role
Probabilities

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Reaction Dynamics
$O(^1D)+H_2$,HD
Wavepacket Method
P.E. Surfaces
Probabilities
Product States

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Reaction Dynamics
$OH+HCOOCH_3$
Rate Constant
Channels

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Reaction Dynamics
$OH+C_2H_6$
$OH+C_2H_5F,C_2H_5Cl$
VTST
Tunneling
Rate Constants

41. CHEMICAL KINETICS - GENERAL

(See also Section 42 for Laser Induced Reactions)

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Oscillations
Nonlinear Dynamics
Monograph

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Flame/
Electric Discharge
Consequences
Breakdown
Excited States
Modeling

(83626) Atmospheric Chemistry, CH_4/CO/OH System, Concentration/Isotopic Relationships
Isotopic Variations

(83981) Kinetic Modeling, Ar_2^* Reactions
Ar Discharge

84096. Min, Z., R.W. Quandt, T.-H. Wong and R. Bersohn, "The CO Product of the Reaction of $O(^3P)$ with CH_3 Radicals," *J. Chem. Phys.* 111, 7369-7372 (1999).
CH_3+O
CO(v,J) Secondary
Product Channel
Mechanism

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CH_3NO_2,CH_3ONO/H
Product Radicals
Stabilities
Dissociation
Channels

84098. Hadrich, S., B. Pfelzer and J. Uhlenbusch, "Coherent Anti-Stokes Raman Scattering Applied to Hydrocarbons in a Microwave Excited Process Plasma," *Plasma Chem. Plasma Process.* 19, 91-109 (1999).
CH_4
Microwave
Discharge
CARS Monitor
CH_4,CH_3,H_2
T,Densities

84099.	Balucani, N., O. Asvany, A.H.H. Chang, S.H. Lin, Y.T. Lee, R.I. Kaiser, H.F. Bettinger, P.v.R. Schleyer and H.F. Schaefer III, "Crossed Beam Reaction of Cyano Radicals with Hydrocarbon Molecules. II. Chemical Dynamics of 1-Cyano-1-methylallene ($CNCH_3CCCH_2$;X^1A') Formation from Reaction of $CN(X^2\Sigma^+)$ with Dimethylacetylene $CH_3CCCH_3(X^1A'_1)$," *J. Chem. Phys.* 111, 7472-7479 (1999).	$CN+C_2(CH_3)_2$ Crossed Beam Dynamics Measurements
84100.	Balucani, N., O. Asvany, A.H.H. Chang, S.H. Lin, Y.T. Lee, R.I. Kaiser, H.F. Bettinger, P.v.R. Schleyer and H.F. Schaefer III, "Crossed Beam Reaction of Cyano Radicals with Hydrocarbon Molecules. I. Chemical Dynamics of Cyanobenzene (C_6H_5CN;X^1A_1) and Perdeutero Cyanobenzene (C_6D_5CN;X^1A_1) Formation from Reaction of $CN(X^2\Sigma^+)$ with Benzene $C_6H_6(X^1A_{1g})$ and d_6-Benzene $C_6D_6(X^1A_{1g})$," *J. Chem. Phys.* 111, 7457-7471 (1999).	$CN+C_6H_6$ $CN+C_6D_6$ Crossed Beam Dynamics Measurements
84101.	Matsumoto, H., S. Tanabe, K. Okitsu, Y. Hayashi and S.L. Suib, "Profiles of Carbon Dioxide Decomposition in a Dielectric-Barrier Discharge Plasma System," *Bull. Chem. Soc. Jpn.* 72, 2567-2571 (1999).	CO_2 Dissociation Electric Discharge
84102.	Min, Z., T.-H. Wong, R. Quandt and R. Bersohn, "The Reactions of $O(^3P)$ with Alkenes: The Formyl Radical Channel," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 10451-10453 (1999).	C_2H_4+O HCO Product Small Yields Mechanism
84103.	Butkovskaya, N.I., and D.W. Setser, "Mechanism for the Reaction of Hydroxyl Radicals with Dimethyl Disulfide," *Chem. Phys. Lett.* 312, 37-44 (1999).	$(CH_3)_2S_2+OH,OD$ Evidence for CH_3SH,CH_3SD Primary Products
84104.	Orlando, J.J., G.S. Tyndall and S.E. Paulson, "Mechanism of the OH Initiated Oxidation of Methacrolein," *Geophys. Res. Lett.* 26, 2191-2194 (1999).	$C_3H_5/O_2/OH$ Product Analysis Mechanism
(83928)	CF,CF_2 Products, Diode Laser Absorption, LIF Measurements	C_4F_8 Discharge
(83950)	C_2 Formation, LIF Spectrum, Wall Mechanism	C_4F_8 Discharge
84105.	Malyshev, M.V., V.M. Donnelly, A. Kornblit and N.A. Ciampa, "Percent Dissociation of Cl_2 in Inductively Coupled, Chlorine-Containing Plasmas," *J. Appl. Phys.* 84, 137-146 (1998).	Cl_2 BCl_3/Cl_2 Plasma Discharge % Dissociation
84106.	Malyshev, M.V., V.M. Donnelly and S. Samukawa, "Ultrahigh Frequency versus Inductively Coupled Chlorine Plasmas: Comparisons of Cl and Cl_2 Concentrations and Electron Temperatures Measured by Trace Rare Gases Optical Emission Spectroscopy," *J. Appl. Phys.* 84, 1222-1230 (1998).	Cl,Cl_2,e^-,T_e Densities Cl_2 Discharges Emission Spectra Xe Trace Addition
84107.	Stevefelt, J., "Calculation of Atomic Recombination in a Decaying High Temperature Hydrogen Gas Column," *Can. J. Chem.* 77, 518-522 (1999).	H-Atom Recombination Cooling Plasma Decay Profiles

84108.	Harris, S.A., S.D. Wiediger and P.R. Brooks, "Electron Transfer to SF_6 and Oriented CH_3Br," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 10035-10041 (1999).	‘Hot' $K+CH_3Br,O_2$ ‘Hot' $K+SF_6$ Product Ions Orientation Effects
84109.	Akermark, T., J.-J. Ganem, I. Trimaille and S. Rigo, "Reactions in the System O_2-NO-N_2O in a Conventional Furnace. II. Chemical Reactions Between O_2 and NO," *J. Electrochem. Soc.* 146, 4586-4589 (1999).	NO/O_2 Heated Furnace NO_2,N_2O Products Isotopic Labeling
(83650)	Stratospheric $^{18}O/^{16}O$, $^{17}O/^{16}O$ Isotopic Ratios, Gaseous Chemical Mechanisms	N_2O
84110.	Savarino, J., and M.H. Thiemens, "Mass Independent Oxygen Isotope (^{16}O, ^{17}O, ^{18}O) Fractionation Found in H_x, O_x Reactions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 9221-9229 (1999).	O Isotopic Fractionations H_2 Discharge/O_2 Product Analysis $H+O_2+M$ Role
(83881)	Crossed Beam, Reactive Scattering, Dynamics, Overview	$O(^3P)+CH_3I,H_2S$
84111.	Falkenstein, Z., "Ozone Formation with (V)UV Enhanced Dielectric Barrier Discharges in Dry and Humid Gas Mixtures of O_2, N_2/O_2, and Ar/O_2" *Ozone Sci. Eng.* 21, 583-603 (1999).	O_3 Formation Air-Like Mixture Discharges VUV Effects
84112.	Bevsek, H.M., M. Ahmed, D.S. Peterka, F.C. Sailes and A.G. Suits, "Direct Detection and Spectroscopy of O_4*," *Faraday Discuss. Chem. Soc.* 108, 131-138 (1997).	O_4* Metastable State Molecular Beam Detection (1+1) REMPI Structure
(83781)	Si Particle Formation	$SiF_4,SiH_4/H_2$ Glow Discharges
(83782) (83783)	Particle Formation, Growth, Measurements	SiH_4 Discharge
(83957)	Product SiH_2 LIF Monitor, SiH_2+SiH_4 Loss Channel	SiH_4 Discharge

84113.	Krier, A., and V.V. Sherstnev, "Powerful Interface Light Emitting Diodes for Methane Gas Detection," *J. Phys. D. Appl. Phys.* 33, 101-106 (2000).	Laser Diode 3.3 μm,3.5 mW Fabrication CH_4 Detector
84114.	Furman, D., B.D. Barmashenko and S. Rosenwaks, "Diode Laser Based Absorption Spectroscopy Diagnostics of a Jet Type $O_2(^1\Delta)$ Generator for Chemical Oxygen/Iodine Lasers," *IEEE J. Quantum Electron.* 35, 540-547 (1999).	O_2(a)/I Chemical Laser O_2(a),H_2O Diode Laser Monitor
84115.	Henriksen, N.E., "Molecular Alignment and Orientation in Short Pulse Laser Fields," *Chem. Phys. Lett.* 312, 196-202 (1999).	Laser Control Molecular Orientation Method
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84118.	Crim, F.F., "Vibrational State Control of Bimolecular Reactions: Discovering and Directing the Chemistry," *Acc. Chem. Res.* 32, 877-884 (1999).	Laser Reaction Control X+HCN,$H_2O(\nu=4)$ H+HOD($5\nu_{OD}$) Cl+HNCO($3\nu_1$) Vibrational Effects
84119.	Gordon, R.J., L. Zhu and T. Seideman, "Coherent Control of Chemical Reactions," *Acc. Chem. Res.* 32, 1007-1016 (1999).	Laser Reaction Control HI,DI Coherent Phase Method
84120.	Frishman, E., M. Shapiro and P. Brumer, "Optimized Imploding Waves in the Coherent Control of Bimolecular Processes: Atom-Rotor Scattering," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 10333-10342 (1999).	Laser Control H_2,HD+Ar Rotational Excitation Sculpted Waveform Method Enhanced Cross Sections

84121.	Kuhn, A., S. Steuerwald and K. Bergmann, "Coherent Population Transfer in NO with Pulsed Lasers: The Consequences of Hyperfine Structure, Doppler Broadening and Electromagnetically Induced Absorption," *Eur. Phys. J. D* 1, 57-70 (1998).	NO(v,J) Population Transfer Method 2 Delayed Laser Pulses
84122.	Hoki, K., Y. Ohtsuki, H. Kono, Y. Fujimura and S. Koseki, "Quantum Control of the Photodissociation of Sodium Iodide," *Bull. Chem. Soc. Jpn.* 72, 2665-2671 (1999).	Laser Control $NaI+h\nu$ Optional Neutral Products Method
(83868)	BaO(A) Lifetime, Quenching, Plume Measurements	Laser Ablation $BaTiO_3$,YBCO
(84199)	Intense Pulsed CN Beam Source, General Method	Laser Ablation Graphite
(83797)	C_n, n=1-30 Formation, TOF Mass Analysis, Distributions	Laser Ablation Graphite
84123.	Mao, S.S., X. Mao, R. Greif and R.E. Russo, "Dynamics of an Air Breakdown Plasma on a Solid Surface during Picosecond Laser Ablation," *Appl. Phys. Lett.* 76, 31-33 (2000).	ps Laser Ablation Plume Cu Target 1.06 μm e^- Densities
(83947)	Product YO Absorption, Xe Lamp	Y_2O_3 Ablation Plume
84124.	Settersten, T., M. Linne, J. Gord and G. Fiechtner, "Density Matrix and Rate Equation Analyses for Picosecond Pump/Probe Combustion Diagnostics," Presented Originally as AIAA Paper 98-0306 at the *36th AIAA Aerospace Sciences Meeting*, Held in Reno NV, January 1998, *AIAA J.* 37, 723-731 (1999).	Laser Diagnostics ps Pump/Probe Rate Equation Formalism
84125.	Farmanara, P., O. Steinkellner, M.T. Wick, M. Wittmann, G. Korn, V. Stert and W. Radloff, "Ultrafast Internal Conversion and Photodissociation of Molecules Excited by Femtosecond 155 nm Laser Pulses," *J. Chem. Phys.* 111, 6264-6270 (1999).	fs Laser Absorption 155 nm Pump/Probe CS_2,C_2H_4,$C_2H_{4-n}Cl_n$ C_6H_6,H_2O(A) NO,O_2(B) fs Decay Rates
84126.	Zhong, D., T.M. Bernhardt and A.H. Zewail, "Femtosecond Real-Time Probing of Reactions. XXIV. Time, Velocity and Orientation Mapping of the Dynamics of Dative Bonding in Bimolecular Electron Transfer Reactions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 10093-10117 (1999).	fs Reaction Probe $ICl,I_2+(CH_3)_2CO$ $ICl,I_2+C_6H_6$ $ICl,I_2+(C_2H_5)_2S$ $ICl,I_2+C_4H_8O_2$ Charge Transfer Dynamics

84127. Ermoshin, V.A., A.K. Kazansky and V. Engel, "Quantum-Classical Molecular Dynamics Simulation of Femtosecond Spectroscopy on I_2 in Inert Gases: Mechanisms for the Decay of Pump-Probe Signals," *J. Chem. Phys.* 111, 7807-7817 (1999). — fs Pump/Probe; I_2(B-X); Vibrational Motion Theory

(83558) As, Cu, Sb, Se Detection Sensitivities, C_2H_2/O_2, Air Flames — Laser Enhanced Ionization

84128. Schick, C.P., S.D. Carpenter and P.M. Weber, "Femtosecond Multiphoton Ionization Photoelectron Spectroscopy of the S_2 State of Phenol," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 10470-10476 (1999). — $C_6H_5OH(S_2)$; fs 2-Photon Ionization/PES; S_2 Lifetime; Ionic (A,X) States

(83912) Gasoline Vapor Monitor, Fiber Optic Probe — REMPI,$C_6H_5CH_3$

(83911) Mass Analyzer, Aromatic Hydrocarbon Monitor, Supersonic Jet — fs MPI

(84015) fs MPD/MPI, Laser Control, Pulse Shaper Method — MPI,$Fe(CO)_5$

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43. P.E. CURVES/SURFACES/ENERGY LEVELS

(See also Section 26 for Spectral Aspects and Section 40 for Surface Dynamics)

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84132. Jost, R., M. Joyeux, S. Skokov and J. Bowman, "Vibrational Analysis of HOCl up to 98% of the Dissociation Energy with a Fermi Resonance Hamiltonian," *J. Chem. Phys.* 111, 6807-6820 (1999). — Vibrational Levels; HOCl; Analysis; Assignments; Mode Behaviors

84133. Huang, S.-W., and T. Carrington Jr., "A Comparison of Filter Diagonalization Methods with the Lanczos Method for Calculating Vibrational Energy Levels," *Chem. Phys. Lett.* 312, 311-318 (1999).

Vibrational Energy Levels
H_2O
High Lying
Calculation Method

84134. Acioli, P.H., L.S. Costa and F.V. Prudente, "Quantum Monte Carlo Study of Rovibrational States Utilizing Rotating Wavefunctions: Application to H_2O," *J. Chem. Phys.* 111, 6311-6315 (1999).

v,J Energy Levels
H_2O
Calculation Method
Accuracies

84135. Szalay, V., "Iterative and Direct Methods Employing Distributed Approximating Functionals for the Reconstruction of a Potential Energy Surface from Its Sample Values," *J. Chem. Phys.* 111, 8804-8818 (1999).

P.E. Surface
Construction Method

84136. Thompson, W.H., "On Obtaining Reactive Potential Energy Surfaces from Transition State Photodetachment Spectra. I. Sensitivity Analysis," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 9500-9505 (1999).

P.E. Surfaces
Photodetachment
Experimental Data
Inversion
Sensitivity Analysis

84137. Thompson, W.H., "On Obtaining Reactive Potential Energy Surfaces from Transition State Photodetachment Spectra. II. Inversion of Spectra in Model Systems," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 9506-9511 (1999).

P.E. Surfaces
Photodetachment
Spectral Inversion Method

84138. Gardner, D.O.N., and L. von Szentpaly, "Valence State Atoms in Molecules. V. Universal Scaling of the Inner Branch of Fifty RKR Potential Energy Curves: Comparison of the Valence State, Morse and Rydberg Curves," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 9313-9322 (1999).

P.E. Curves
Inner Branch
Universal Fit
50 Diatomics
D_e Predictor

84139. Reddy, R.R., Y.N. Ahammed, K.R. Gopal, P.A. Azeem and S. Anjaneyulu, "RKRV Potential Energy Curves, Dissociation Energies, γ-Centroids and Franck-Condon Factors of YO, CrO, BN, ScO, SiO and AlO Molecules," *Astrophys. Space Sci.* 262, 223-240 (1999).

P.E. Curves
AlO(D,B-X)
BN(A-X)
CrO,ScO,YO(B-X)
SiO(E-X)
F.C. Factors
r-Centroids
D_0

84140. Leung, A.W.K., and W.H. Breckenridge, "An ab Initio Study of the Ground States and Some Excited States of BeRg, Be^+Rg, and $Be^{+2}Rg$ van der Waals Complexes (Rg=He,Ne)," *J. Chem. Phys.* 111, 9197-9202 (1999).

P.E. Curves
BeRg,Be^+Rg
Rg=He,Ne
Low-lying States
Spectral Constants
D_e
Calculations

84141. Manaa, M.R., and L.E. Fried, "Intersystem Crossings in Model Energetic Materials," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 9349-9354 (1999).

P.E. Surfaces
CH_3NO_2, HNO_3
NH_2NO_2
^{1,3}Crossings

84142. Li, Y., and J.S. Francisco, "A CASSCF-MRCI Study on the Low-lying Excited States of CH_3OCl," *J. Chem. Phys.* 111, 8384-8388 (1999).

P.E. Curves
CH_3OCl
Low-lying States
Energies
$2^1A'$,$1^1A''$-X)
Transitions
Calculations

(84039) P.E. Surfaces, Singlet/Triplet States, Unimolecular Dissociation, Rate Constants, RRKM Calculations

$^{1,3}CH_3S^+$

84143. Panten, D., G. Chambaud, P. Rosmus and P.J. Knowles, "Rovibronic States of the $X^2\Pi$ State of CCO^-," *Chem. Phys. Lett.* 311, 390-394 (1999).

P.E. Functions
C_2O^-(X)
v,J Energy Levels
Spectral Constants
A-State Lifetime
Calculations

(84048) P.E. Surfaces, Low-lying States, Linear/Bent Structures, Isomerization, Calculations

C_3, C_3^-

84144. Peterson, K.A., S. Skokov and J.M. Bowman, "A Theoretical Study of the Vibrational Energy Spectrum of the HOCl/HClO System on an Accurate ab Initio Potential Energy Surface," *J. Chem. Phys.* 111, 7446-7456 (1999).

P.E. Surfaces
HOCl,HClO
Vibrational
Energy Levels
Accuracies
Transition
Probabilities

(84053) P.E. Surfaces, Unimolecular Dissociation, Isomerization, Barriers, D(HOSO)

HSO_2, HOSO
HOOS

84145. Abrol, R., N. Sathyamurthy and M.K. Harbola, "Reduced Potential Energy Curves for Diatomic Molecules and Their Respective Cations," *Chem. Phys. Lett.* 312, 341-345 (1999).

Reduced
P.E. Curves
H_2, H_2^+
Li_2, Li_2^+, N_2, N_2^+
Ion/Neutral
Similarities

84146. Bettens, R.P.A., T.A. Hansen and M.A. Collins, "Interpolated Potential Energy Surface and Reaction Dynamics for $O(^3P)+H_3^+(^1A'_1)$ and $OH^+(^3\Sigma^-)+H_2(^1\Sigma_g^+)$," *J. Chem. Phys.* 111, 6322-6332 (1999).

P.E. Surface
H_3O^+
$O+H_3^+/H_2O^++H/$
OH^++H_2
Dynamics
Rate Constants

84147. van Mourik, T., and T.H. Dunning, Jr., "A New ab Initio Potential Energy Curve for the Helium Dimer," *J. Chem. Phys.* 111, 9248-9258 (1999).

P.E. Curve
He_2
Well Depth

84148. Margulis, C.J., D.A. Horner, S. Bonella and D.F. Coker, "Vibrational Dynamics of the I_3 Radical: A Semiempirical Potential Surface and Semiclassical Calculation of the Anion Photoelectron Spectrum," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 9552-9563 (1999).

P.E. Surface
I_3
I_3^- PES
Calculations

84149. Christiansen, P.A., T.M. Moffett and G.A. DiLabio, "Potential Curves for the Mg^+Rn Complex Including Charge Transfer States," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 8875-8878 (1999).

P.E. Curves
Mg^+Rn
Rg Comparisons
Low-lying States
Spectral Constants
Calculations

84150. Alexander, M.H., "A New, Fully ab Initio Investigation of the $NO(X^2\Pi)Ar$ System. I. Potential Energy Surfaces and Inelastic Scattering," *J. Chem. Phys.* 111, 7426-7434 (1999).

P.E. Surfaces
NO.Ar
Well Depth
NO(J)+Ar
Spin-Orbit
Changing
Cross Sections

84151. Alexander, M.H., "A New, Fully ab Initio Investigation of the $ArNO(X^2\Pi)$ System. II. Bound States of the Ar-NO Complex," *J. Chem. Phys.* 111, 7435-7439 (1999).

P.E. Surface
NO.Ar
Bound States
Energy Level
Calculations

84152. Brown, A., P. Jimeno and G.G. Balint-Kurti, "Photodissociation of N_2O. I. Ab Initio Potential Energy Surfaces for the Low-lying Electronic States X^1A', $2^1A'$ and $1^1A''$," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 11089-11095 (1999).

P.E. Surfaces
$N_2O(1^1A'',2^1A',X^1A')$
Conical Intersection
Absorption
Transitions

84153. Almazor, M.-L., O. Dulieu, M. Elbs, E. Tiemann and F. Masnou-Seeuws, "How to Get Access to Long Range States of Highly Excited Molecules," *Eur. Phys. J. D* 5, 237-242 (1999).

P.E. Curves
$Na_2(6^1\Sigma_g^+)$
Secondary Well
Populating
Possibilities

84154. Kalemos, A., and A. Mavridis, "On the Electronic Structure of ScB^+: Ground and Low-lying Excited States," *Adv. Quantum Chem.* 32, 69-91 (1999).

P.E. Curves
ScB^+
Low-lying States
Spectral Constants
D_e
Calculations

44. ATOMIC/MOLECULAR STRUCTURES

(See also Section 26 for Spectrally Measured Structures)

84155.	Zheng, X., Z. Wang and A. Tang, "Equilibrium Structure and Stability of AlC_n(n=2,3) and AlC_nN(n=1,2) Species," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 9275-9279 (1999).	Structural Calculations AlC_2 ,AlC_3 AlCN,AlC_2N Geometries Frequencies Stabilities
84156.	Feng, P.Y., and K. Balasubramanian, "Spectroscopic Properties of Al_2P_2 , $Al_2P_2^+$ and $Al_2P_2^-$ and Comparison with Their Ga and In Analogs," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 9093-9099 (1999).	Structural Calculations Al_2P_2 ,$Al_2P_2^{\pm}$ Low-lying States Geometries
84157.	Alder, R.W., M.E. Blake and J.M. Oliva, "Diaminocarbenes; Calculation of Barriers to Rotation about $C_{carbene}$-N Bonds, Barriers to Dimerization, Proton Affinities and ^{13}C NMR Shifts," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 11200-11211 (1999).	Structural Calculations $C(NH_2)_2$,$CH^+(NH_2)_2$ $C(N(CH_3)_2)_2$ $CH^+(N(CH_3)_2)_2$ $CLi^+(NH_2)_2$ $CLi^+(N(CH_3)_2)_2$ Dimerization PAS
(84048)	Linear/Bent Structures, P.E. Surfaces, Low-lying States, Isomerization, Calculations	C_3 ,C_3^-
84158.	Saeh, J.C., and J.F. Stanton, "Application of an Equation-of-Motion Coupled Cluster Method Including Higher-Order Corrections to Potential Energy Surfaces of Radicals," *J. Chem. Phys.* 111, 8275-8285 (1999).	Structural Calculations *c*-C_3H NO_2(A,X) Coupled Cluster Method
84159.	Cioslowski, J., G. Liu and D. Moncrieff, "Theoretical Thermochemistry of the 1-Buten-3-yn-1-yl Radical and Its Chloro Derivatives," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 11465-11468 (1999).	Structural Calculations $CHCCHCH_2$ Geometries D,ΔH_f
84160.	Weber, P., and J.R. Reimers, "Ab Initio and Density Functional Calculations of the Energies of the Singlet and Triplet Valence Excited States of Pyrazine," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 9821-9829 (1999).	Structural Calculations *c*-$C_4H_4N_2$ ^{1,3}Low-lying States Excitation Energies

84161. Weber, P., and J.R. Reimers, "Ab Initio and Density Functional Calculations of the Vibrational Structure of the Singlet and Triplet Excited States of Pyrazine," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 9830-9841 (1999).

Structural Calculations
c-$C_4H_4N_2$
^{1,3}Low-lying States
Vibrational Frequencies

84162. Chipman, D.M., "Structure and Properties of *p*-Aminophenoxyl Radical," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 11181-11187 (1999).

Structural Calculations
$NH_2C_6H_4O$
Geometry
Frequencies

84163. Filatov, M., and S. Shaik, "Tetramethyleneethane Diradical: Experiment and Density Functional Theory Reach an Agreement," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 8885-8889 (1999).

Structural Calculations
$C_2(CH_2)_4$
Diradical
^{1,3}States
Frequencies

84164. Li, Q., G. Li, W. Xu, Y. Xie and H.F. Schaefer III, "Structures, Thermochemistry, and Electron Affinities of the Germanium Fluorides, GeF_n/GeF_n^-(n=1-5)," *J. Chem. Phys.* 111, 7945-7953 (1999).

Structural Calculations
GeF_n, GeF_n^-
n=1-5
Frequencies
Geometries
D,EAS

84165. Ceotto, M., F.A. Gianturco and D.M. Hirst, "Protonated Ozone: Structure, Energetics and Nonadiabatic Effects," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 9984-9994 (1999).

Structural Calculations
HO_3^+
Geometries
PA(O_3)

84166. Li, X., and L.-S. Wang, "Electronic Structure and Chemical Bonding between the First Row Transition Metals and C_2: A Photoelectron Spectroscopy Study of MC_2^- (M=Sc,V,Cr,Mn,Fe and Co)," *J. Chem. Phys.* 111, 8389-8395 (1999).

Structures
MC_2
Frequencies
Low-lying States
EAS
MC_2^-,PES
M=Sc,V,Cr,Mn, Fe,Co

(84193) Structural Calculations, Geometries, Frequencies, ΔH_f

PO_n, n=1-3
HPO_n

45. ENERGY TRANSFER

(See also Section 27 for Electronically Excited State Relaxation Processes)

84167.	Maciejewski, A., M. Milewski and M. Szymanski, "A Method of Determination of Quantum Yields of $S_3 \rightarrow S_2$, $S_3 \rightarrow S_1$, and $S_3 \rightarrow S_0$ Intramolecular Radiationless Transitions," *J. Chem. Phys.* 111, 8462-8468 (1999).	Intramolecular Relaxation $S_3 \rightarrow S_2, S_1, S_0$ Quantum Yields Absorption Fluorescence Phosphorescence Measurement Method
84168.	Franklin, R.E., and G.P. Perram, "Collisional Dynamics of $Bi_2(A0_u^+)$. I. Quantum Resolved Vibrational Energy Transfer for v=0-4," *J. Chem. Phys.* 111, 5757-5763 (1999).	Vibrational Relaxation Bi_2(A,v=1-4)+Rg Rate Constants Measurements
(83826)	SRL LIF Decay, Rate Constants, Magnetic and Microwave Field Effects	$(COF)_2, (^1A_u)$
84169.	Wall, M.C., A.E. Lemoff and A.S. Mullin, "Unraveling the Energy Dependence in Large ΔE(V→RT) Energy Transfer: Separation of ΔE and Probability in the Collisional Relaxation of Highly Vibrationally Excited Pyrazine (E_{vib}=36000 to 41000 cm^{-1}) by CO_2," *J. Chem. Phys.* 111, 7373-7382 (1999).	V-RT Transfer c-$C_4H_4N_2 + CO_2$ Highly Excited Large ΔE Collisions
84170.	Heidelbach, C., V.S. Vikhrenko, D. Schwarzer, I.I. Fedchenia and J. Schroeder, "Molecular Dynamics Simulation of Vibrational Energy Relaxation of Highly Excited Molecules in Fluids. III. Equilibrium Simulations of Vibrational Energy Relaxation of Azulene in Carbon Dioxide," *J. Chem. Phys.* 111, 8022-8033 (1999).	Vibrational Relaxation c-$C_{10}H_8 + CO_2$ Intermode Couplings Theory
84171.	Clare, S., A.J. Marks and A.J. McCaffery, "Rotational and Vibrotational Transfer in H*-CO_2 Collisions: The Influence of Stereokinematic Restrictions," *J. Chem. Phys.* 111, 9287-9295 (1999).	T-v,J Transfer 'Hot' H+CO_2 Relative Cross Sections
(84029)	Vibrational Relaxation Rate Constants, $CF_2CH_2 + h\nu$, $CF_2CH_2/Cl_2 + h\nu$	HF(v=1-5) HCl(v=1-4)
84172.	McCaffery, A.J., "Quasiresonant Vibration-Rotation Transfer: A Kinematic Interpretation," *J. Chem. Phys.* 111, 7697-7700 (1999).	v,J Relaxation Li_2(A,v,J)+Ne Angular Momentum Model Application

84173.	Islam, M., and I.W.M. Smith, "Rotationally Specific Rates of Vibration-Vibration Energy Exchange in Collisions of $NO(X^2\Pi_{1/2},v=3)$ with $NO(X^2\Pi,v=0)$," *J. Chem. Phys.* 111, 9296-9302 (1999).	V-V Transfer NO(v=3)+NO State-to-State Rate Constants J Propensity
(84150)	Spin-Orbit Changing Collisions, Cross Sections, NO.Ar P.E. Surface, Calculations, Discrepancies	NO(J)+Ar

46. THERMOCHEMISTRY

84174.	Benson, S.W., "New Methods for Estimating the Heats of Formation, Heat Capacities and Entropies of Liquids and Gases," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 11481-11485 (1999).	ΔH_f, C_p, S° Liquids,Gases Group Additivity Calculation Method
(84166)	M=Sc,V,Cr,Mn,Fe,Co, Ion Photoelectron Spectra, MC_2 Structures, Frequencies, Low-lying States	$EA(MC_2)$
(83980)	$Al(^2P_J)+O_2$ Rate Constants, Crossed Beams, Spin-Orbit Effects	$D_0(AlO)$
(84139)	P.E. Curve Construction, Low-lying States, F.C. Factors, *r*-Centroids	$D_0(AlO,BN,CrO)$ $D_0(ScO,SiO,YO)$
84175.	Morosi, G., M. Mella and D. Bressanini, "Quantum Monte Carlo Calculations of Molecular Electron Affinities: First Row Hydrides," *J. Chem. Phys.* 111, 6755-6758 (1999).	EA(BH,BeH,LiH) EA(CH,NH,OH) Calculations
(83809)	B_2N^- Photoelectron Spectra, $B_2N(A,X)$ Spectral Characterizations	$EA(B_2N)$
(84140)	Rg=He,Ne, P.E. Curves, Low-lying States, Spectral Constants, Calculations	$D_e(BeRg,Be^+Rg)$
(83811)	BrO(A-X) FT Ultraviolet Spectrum, Constants, Cross Sections	ΔH_f, $D_0(BrO)$
84176.	Ma, N.L., K.-C. Lau, S.-H. Chien and W.-K. Li, "Thermochemistry of Hydrochlorofluoromethanes Revisited: A Theoretical Study with the Gaussian-3 Procedure," *Chem. Phys. Lett.* 311, 275-280 (1999).	ΔH_f, IP,PA $CH_{4-x-y}Cl_xF_y$ Adequacies Deficiencies
84177.	Parkinson, C.J., P.M. Mayer and L. Radom, "An Assessment of Theoretical Procedures for the Calculation of Reliable Radical Stabilization Energies," *J. Chem. Soc., Perkin Trans. II. Phys. Org. Chem.* 2305-2313 (1999).	Relative Bond Strengths CH_2F,CH_2CN,CH_2CF C_3H_5,CH_2CHO CH_2CCN H-Atom Abstractions Calculations

84178.	Chen, E.C.M., N. Welk, E.S. Chen and W.E. Wentworth, "Electron Affinity, Gas Phase Acidity, Bond Dissociation Energy and Negative Ion States of Nitromethane," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 9072-9079 (1999).	D,EA(CH_3NO_2) D,EA($C_6H_5CH_2NO_2$) Electron Capture Data Analysis
84179.	Vreven, T., and K. Morokuma, "The Accurate Calculation and Prediction of the Bond Dissociation Energies in a Series of Hydrocarbons Using the IMOMO (Integrated Molecular Orbital+Molecular Orbital) Methods," *J. Chem. Phys.* 111, 8799-8303 (1999).	Bond Energies Hydrocarbons Predictive Method
84180.	Weitzel, K.-M., M. Malow, G.K. Jarvis, T. Baer, Y. Song and C.Y. Ng, "High Resolution Pulsed Field Ionization Photoelectron-Photoion Coincidence Study of CH_4: Accurate 0 K Dissociation Threshold for CH_3^+," *J. Chem. Phys.* 111, 8267-8270 (1999).	$D_0(CH_4, CH_4^+)$ CH_3^+ PFI-PEPICO CH_4 Fragmentation Spectrum
(84157)	Structural Calculations, Dimerization	PA($C(NH_2)_2$) PA($C(N(CH_3)_2)_2$)
(83816)	Pulsed Field Ionization-Photoelectron Spectra, CO^+(X,v=0-42)-CO(X,v=0), Constants, Ionization Potential	$D_0(CO^+)$
84181.	Lu, W., P. Tosi, and D. Bassi, "Guided Ion Beam Investigation of the Reaction CO^++CO: C-O Bond Activation and C-C Bond Formation," *J. Chem. Phys.* 111, 8852-8856 (1999).	$\Delta H_f(C_2^+, C_2O^+)$ $D_0(C_2^+)$ CO^++CO Reactive Channels Threshold Measurements
(83822)	$C_2H_2^+$(D,C,B,A,X) Photoionized Product States, Cross Sections, Spectral Analysis, Calculations	IP(C_2H_2)
84182.	Alconcel, L.S., H-J. Deyerl, V. Zengin and R.E. Continetti, "Structure and Energetics of Vinoxide and the X($^2A''$) and A($^2A'$) Vinoxy Radicals," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 9190-9194 (1999).	EA(C_2H_3O) (A,X) Energy Splitting PES,$C_2H_3O^-$ Measurements
(84045)	Structural Calculations, Reaction Enthalpy Calculations, PAN Dissociation Pathways	$\Delta H_f(CH_3C(O)O)$ ΔH_f(PAN,$CH_3C(O)O_2$)
(84010)	C_2H_5OH, C_2H_5OD+hν, Channels, Product Energies	D(C_2H_5OH,C_2H_5OD)
(84159)	Structural Calculations, Geometries	D,ΔH_f($CHCCHCH_2$)
84183.	Lindh, R., A. Bernhardsson and M. Schutz, "Benzyne Thermochemistry: A Benchmark ab Initio Study," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 9913-9920 (1999).	D(*c*-C_6H_4) ^{1,3}Energy Splitting Calculations

84184.	Kim, J.B., P.G. Wenthold and W.C. Lineberger, "Ultraviolet Photoelectron Spectroscopy of *o-, m-,* and *p*-Halobenzyl Anions," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 10833-10841 (1999).	EA($XC_6H_4CH_2$) D($XC_6H_4CH_3$) Anion PES Vibrational Structure X=F,Cl,Br
84185.	Mo, O., M. Yanez, M.V. Roux, P. Jimenez, J.Z. Davalos, M.A.V. Ribeiro da Silva, M.d.D.M.C. Ribeiro da Silva, M.A.R. Matos, L.M.P.F. Amaral, A. Sanchez-Migallon, P. Cabildo, R. Claramunt, J. Elguero and J.F. Liebman, "Enthalpies of Formation of N-Substituted Pyrazoles and Imidazoles," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 9336-9344 (1999).	ΔH_f 4 Azoles Calorimetry Measurements
(83467)	Epoxy, Phenolic, Imide, Vinyl Ester Composites, Auto-ignition Temperatures	$\Delta H_{Combustion}$
84186.	Vahlas, C., A. Kacheva, M.L. Hitchman and P. Rocabois, "Thermodynamic Study of the Formation of C_{60} and C_{70} by Combustion or Pyrolysis," *J. Electrochem. Soc.* 146, 2752-2761 (1999).	C_{60} ,C_{70} Thermodynamic Stabilities C/H/O/Ar C/H/O/F/Ar Calculations
(84164)	n=1-5, Structural Calculations, Frequencies, Geometries	D,EA(GeF_n)
84187.	Ricca, A., and C.W. Bauschlicher Jr., "Heats of Formation for GeH_n (n=1-4) and Ge_2H_n (n=1-6)," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 11121-11125 (1999).	$\Delta H_f(GeH_n)$,n=1-4 $\Delta H_f(Ge_2H_n)$,n=1-6 Calculations
(83875)	He(2^3S)+HNCO,HNCS, Penning Ionization, Photoelectron Spectroscopy Measurements	IP(HNCO,HNCS)
(84053)	Unimolecular Dissociation, Isomerization, P.E. Surfaces, Barriers, HSO_2 , HOSO, HOOS	D(HOSO)
(84147)	P.E. Curve Calculations	$D_e(He_2)$
84188.	Awitor, K.O., L. Bernard, O. Bonnin, B. Coupat, J.P. Fournier and P. Verdier, "Formation of Mercury Chloride, Hg_2Cl_2 , and Vapor Pressure Measurements," *Can. J. Chem.* 77, 243-248 (1999).	$Hg_2Cl_2(s)$ Vapor Pressures Knudsen Cell Hg,$HgCl_2$ Presence
(84026)	CN Product Velocities, (A-X) Doppler Profiles, ICN+hν Dynamics	D(ICN)
(83841)	(B-X) LIF Spectra, Linear, T-Shaped Isomers	$D_0(I_2 .Ar)$
(83842)	OODR Spectra, Constants, P.E. Curves	$D_0(KRb(2^1\Pi,1^1\Pi,X))$

84189.	Chen, Z., and T.P. Hamilton, "Ab Initio Calculation of the Heats of Formation of Nitrosamides: Comparison with Nitramides," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 11026-11033 (1999).	ΔH_f $N(NO)_3$,$NH(NO)_2$ NH_2NO,NH_2NO_2 Calculations
(83990)	Li, Na, K+NO+Ar Rate Constants, RRKM Modeling Analysis	D(NaNO,KNO)
84190.	Chang, E.S., J. Li, J. Zhang, C.-C. Tsai, J. Bahns and W.C. Stwalley, "Theory and Analysis of Sodium Dimer Rydberg States Observed by All-Optical Triple-Resonance Spectroscopy," *J. Chem. Phys.* 111, 6247-6252 (1999).	IP(Na_2),D_0(Na_2^+) Na_2 Rydberg State Analysis
84191.	Archer, D.G., "Thermodynamic Properties of Import to Environmental Processes and Remediation. II. Previous Thermodynamic Property Values for Nickel and Some of Its Compounds," *J. Phys. Chem. Ref. Data* 28, 1485-1507 (1999).	Thermochemical Values Ni,NiO,$Ni(OH)_2$ $NiCl_2$,$NiSO_4$,$NiCO_3$ Solid Phase Salts Evaluation
84192.	Taniguchi, N., K. Takahashi, Y. Matsumi, S.M. Dylewski, J.D. Geiser and P.L. Houston, "Determination of the Heat of Formation of O_3 using Vacuum Ultraviolet Laser Induced Fluorescence Spectroscopy and Two-Dimensional Product Imaging Techniques," *J. Chem. Phys.* 111, 6350-6355 (1999).	$\Delta H_f(O_3)$ $O_3/O(^1D)+O_2(a)$ Threshold VUV LIF REMPI Imaging Method
(84165)	Structural Calculations HO_3^+, Geometries	PA(O_3)
84193.	Bauschlicher Jr., C.W., "Heats of Formation for PO_n and PO_nH (n=1-3)," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 11126-11129 (1999).	$\Delta H_f(PO_n)$ $\Delta H_f(HPO_n)$ n=1-3 Geometries Frequencies Calculations
(83857)	VUV Absorption Spectrum, (C,B,A,X) Ionic Limits	IP(PbO)
84194.	Martin, J.M.L., "Heat of Atomization of Sulfur Trioxide, SO_3: A Benchmark for Computational Thermochemistry," *Chem. Phys. Lett.* 310, 271-276 (1999).	$\Delta H_{Atomization}$ SO_3 Benchmark Calculations
(84154)	P.E. Curves, Low-lying States, Spectral Constants, Calculations	$D_e(ScB^+)$
84195.	Capone, F., Y. Colle, J.P. Hiernaut and C. Ronchi, "Mass Spectrometric Measurement of the Ionization Energies and Cross Sections of Uranium and Plutonium Oxide Vapors," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 10899-10906 (1999).	D,IP(UO,UO_2,UO_3) D,IP(PuO,PuO_2) Measurements

47. EXPERIMENTAL METHODS

84196.	Friedrich, B., and D. Herschbach, "Manipulating Molecules via Combined Static and Laser Fields," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 10280-10288 (1999).	Beam Orientation Static/Laser Fields Linear Molecule Manipulation Methods
84197.	Hain, T.D., R.M. Moision and T.J. Curtiss, "Hexapole State-Selection and Orientation of Asymmetric Top Molecules: CH_2F_2," *J. Chem. Phys.* 111, 6797-6806 (1999).	Molecular Beam Orientation CH_2F_2,CH_2O Hexapole Focusing Method
84198.	Larsen, J.J., H. Sakai, C.P. Safvan, I. Wendt-Larsen and H. Stapelfeldt, "Aligning Molecules with Intense Nonresonant Laser Fields," *J. Chem. Phys.* 111, 7774-7781 (1999).	Laser Beam Alignment Method CH_3I,CS_2,ICl C_6H_5I,I_2 Efficiencies
84199.	Kaiser, R.I., J.W. Ting, L.C.L. Huang, N. Balucani, O. Asvany, Y.T. Lee, H. Chan, D. Stranges and D. Gee, "A Versatile Source to Produce High Intensity, Pulsed Supersonic Radical Beams for Crossed Beam Experiments: The Cyanogen Radical $CN(X^2\Sigma^+)$ as a Case Study," *Rev. Sci. Instrum.* 70, 4185-4191 (1999).	Intense Pulsed Beam Source CN C Laser Ablation General Method
84200.	Gupta, M., and D. Herschbach, "A Mechanical Means to Produce Intense Beams of Slow Molecules," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 10670-10673 (1999).	Molecular Beams Low Velocity Method Xe;O_2/Xe CH_3F/Xe
(83908)	Coupled Gas Chromatography, Molecular Beam/Mass Spectrometer Technique, Complementary Aspects	Flame Monitor

48. MISCELLANEOUS

84201.	Wilson, K.R., "Summing Up," *J. Phys. Chem. A. Mol., Spectrosc., Kinetics* 103, 10022-10034 (1999).	K.R. Wilson Biography Bibliography
84202.	Cropper, W.H., *"Mathematica Computer Programs for Physical Chemistry,"* 246 pp., Springer-Verlag, New York (1998).	Computer Codes Physical Chemistry Applications 140 Program Descriptions